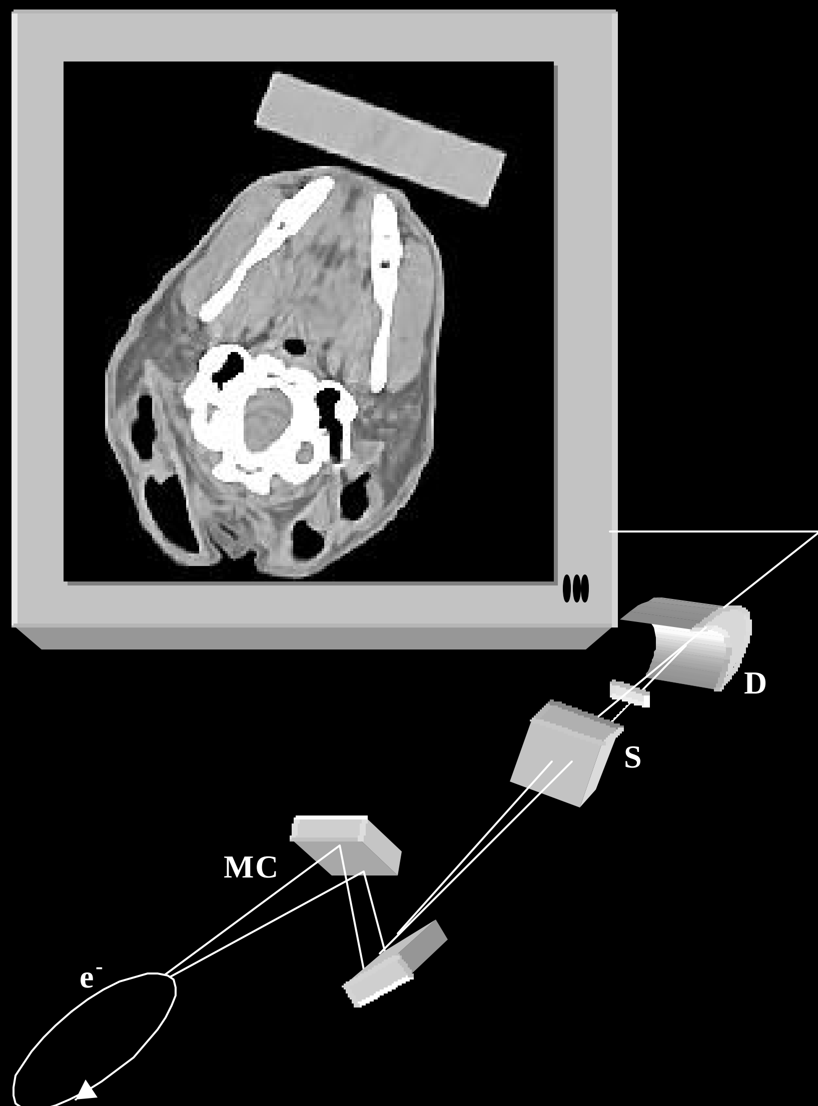
LABORATORY TECHNOLOGY RESEARCH

Abstracts of FY 1999 Projects



U. S. Department of Energy
Office of Science
Advanced Scientific Computing Research
Technology Research Division
Germantown, MD 20874-1290

About the Cover

The cover is a transmission x-ray computed tomography (CT) image of a 2-mm slice of the lower portion of the head of an anesthetized rabbit. The picture was taken with the monochromatic-beam CT scanner "Multiple Energy Computed Tomography (MECT)" at the X17B2 superconducting beamline of the National Synchrotron Light Source (NSLS) at Brookhaven National Laboratory (BNL). Also depicted is the x-ray fan beam from the electron storage ring (e^-), directed to a monochromator (MC), through the sample (S), and onto a scintillator/detection arrangement (D). Compared to a conventional CT image of the same rabbit, when corrected for equal radiation-absorbed dose to the animal, the MECT picture has significantly higher soft-tissue contrast, spatial resolution, and much lower image noise. MECT's narrow energy bandwidth and tunable energy make it the world's best CT scanner. These features allow use of optimal beam energy for a given subject size or application, producing images free of beam-hardening artifacts. Thus, one may clearly distinguish between fatty areas (black), muscle (grey), and bone (white). MECT will be used to evaluate gadolinium-based contrast agents that are being developed in this CRADA between Schering AG and BNL. For more information, see abstract No. 40.

TABLE OF CONTENTS

Laboratory Technology Research Program Overview

The Laboratory Technology Research (LTR) program supports high-risk, multidisciplinary research partnerships to investigate challenging scientific problems whose solutions have promising commercial potential. These partnerships capitalize on two great strengths of our country: the world-class basic research capability of the DOE Office of Science (SC) national laboratories and the unparalleled entrepreneurial spirit of American industry.

A distinguishing feature of the SC national laboratories is their ability to integrate broad areas of science and engineering in support of national research and development goals. The LTR program leverages this strength for the Nation's benefit by fostering partnerships with U.S. industry. The partners jointly bring technology research to a point where industry or the Department's technology development programs can pursue final development and commercialization.

Collaborative research projects supported by the LTR program are partnerships: the program funds only the national laboratory's research, while the industrial partner supports its research and often provides equipment, funds, or supplies to the laboratory. Thus, a laboratory and its industrial partners can explore scientific and technical approaches that would be too risky for industry to undertake alone. Such work leverages the resources of both partners, since each frequently has unique and complementary facilities and expertise.

The LTR program enhances opportunities to pursue technology research that is of value to industry, complements basic research program goals, and seeks to enhance public benefit from investment in scientific research at the national laboratories.

The scientific impact of the LTR program has already been dramatic. Since its inception in 1992, the program's technologies have won 25 R&D-100 Awards, 18 Federal Laboratory Consortium Awards, and 11 other awards, such as those from Popular Science and Discover magazines. The record of R&D-100 Awards exemplifies the steadily increasing success of these cooperatively developed technologies. In addition, LTR principal investigators have earned ten awards for their work, such as the American Physical Society sponsored James C. McGroody Prize and the Biemann Medal of the American Society for Mass Spectroscopy.

LTR projects explore the applications of basic research advances relevant to DOE's mission over a full range of scientific disciplines. The program presently emphasizes three critical areas of mission-related research: advanced materials, intelligent processing and manufacturing research, and environmental and biomedical research.

Projects supported by the LTR program are conducted by ten SC national laboratories: Argonne, Brookhaven, Lawrence Berkeley, Oak Ridge, and Pacific Northwest National Laboratories, and the following five laboratories, which were reinstated into the LTR program at the beginning of FY1999: Ames Laboratory, Fermi National Accelerator Laboratory, Princeton Plasma Physics Laboratory, Stanford Linear Accelerator Center, and Thomas Jefferson National Accelerator Facility.

Laboratory Technology Research Program Focus Areas

Advanced Materials

The Advanced Materials portion of the LTR program will provide a strong foundation for advances in many areas of science and technology including energy, transportation, manufacturing, health, and the environment. Using synthesis, processing, and characterization techniques and advanced computational tools for design and modeling coupled with the integration of basic and applied disciplines, this research will result in the improvement of existing materials and the development of new materials and knowledge of their properties. Research focuses on a broad range of materials problems related to ceramics and composites, metals and alloys, surfaces and thin films, nanomaterials, polymers and biomaterials, and superconducting materials. Results support DOE missions in basic science, energy efficiency, fossil energy, fusion energy, environmental management, and national security. The research is intended to complement, enhance, and leverage existing DOE materials programs through research partnerships. Advanced materials research focuses on four major subtopics.

Design of Materials: Emphasis is placed on modeling and characterization; alloying and doping; composite and functional graded materials; biomaterials; and nanostructures. This includes materials that respond to external stimuli, such as shape memory alloys, magneto-resistant, piezoelectric, and electro-rheologic materials.

Advanced Synthesis and Characterization Technologies: Emphasis is placed on advanced techniques such as ion, plasma, laser, and MBE techniques and environmentally friendly processing techniques that reduce waste and/or energy consumption.

Films and Coatings: Emphasis is placed on surface modification, corrosion and wear resistance, and multilayered films.

Energy Conversion and Storage: Emphasis is placed on materials that can be used for the manufacture and processing of fuels as well as the development of materials useful in the construction and improved performance of batteries and fuel cells.

Intelligent Processing and Manufacturing Research

Intelligent Processing and Manufacturing Research (IPMR) is a multidisciplinary activity which integrates and builds upon the results of DOE basic research to develop new and advanced processing and manufacturing technologies required to meet DOE missions. The goal of IPMR is to perform technology research projects that apply core DOE laboratory capabilities to advance the state of intelligent processing and manufacturing. To meet this goal, research is conducted on a range of technology areas that include advanced sensors and controllers, computational technologies, and algorithms coupled with manufacturing processes. Research projects typically have applications in multiple manufacturing sectors and support DOE missions in science and technology, as well as energy and environment. IPMR projects also benefit national initiatives related to manufacturing such as Technologies Enabling Agile Manufacturing (TEAM), Next Generation Manufacturing (NGM), and the Partnership for a New Generation of Vehicles (PNGV). IPMR focuses on three major subtopics.

Intelligent Design: Emphasis is placed on modeling and simulation and on rapid prototyping.

Intelligent Manufacturing Processes: Emphasis is placed on joining; forming, forging, and casting; and microfabrication.

Enabling Technologies: Emphasis is placed on intelligent measurements, intelligent controls, and agile automation.

Laboratory Technology Research Program Focus Areas

Environmental and Biomedical Research

A new generation of environmental and biomedical technologies is needed that will enhance the general population's quality of life. This research area combines environmental technologies such as: pollution prevention, efficient resource use, and industrial ecology as well as biomedical technologies including radiopharmaceuticals and biomaterials. Such technologies can help companies become more competitive by lowering resource and energy needs, reducing waste and emissions control costs, and fostering sustainable development while enhancing the general health and well being of the general populace. SC supported programs in biotechnology, chemical and materials sciences, and novel energy concepts provide a fertile ground for further investigation for potential commercial application. Priorities for research in this area stress technologies that emphasize sustainable use of natural resources and avoidance of environmental harm as well as more effective biomaterials and medical technologies. These may include technologies to control and minimize environmental harm (particularly hazardous wastes), biomaterials with improved performance, efficacious radiopharmaceutical delivery systems, as well as environmental monitoring and remediation technologies. Research on environmental and biomedical research focuses on four major subtopics.

Biological and Environmental Technologies: Emphasis is on furthering developments in understanding the microbial and biochemical mechanisms that can contribute to solving complex bioprocessing problems. Topics in molecular biology, biochemistry, microbiology, and remediative biotechnologies fall into this category.

Medical Technologies: Emphasis is placed on health related technologies. Topics in this area include diagnostic technologies, biomaterials, and biomedicine.

Cleaner Industrial Processes: Emphasis is placed on both experimental and computational capabilities in the development of environmentally benign industrial processes. This topic may span a variety of technologies from the application of modeling tools in the development, at the structural level, of new classes of catalysts, to large scale industrial process modeling.

Major Industry Partnerships

These partnerships team scientists and engineers in DOE national laboratories with an industry sector to research generic problems facing that industry. This is divided into two areas: the Advanced Computational Technology Initiative (ACTI) Partnership and the American Textiles (AMTEX) Partnership.

ACTI Partnership: ACTI pursues advanced computational technology for finding, developing, and producing natural gas and oil. This technology is directed towards the discovery of natural gas and oil.

AMTEX Partnership: The mission of AMTEX is to infuse technology into the integrated textile and apparel industry to offset foreign competition from low labor rates. Examples of these technologies are on-line inspection of cloth as it comes off the loom, and providing removable protective coatings for fibers to allow them to survive the weaving process and recovery of oil and gas by supporting borehole seismic, oil recovery, and drilling with the goal of enhanced production.

PROGRAM IMPLEMENTATION

The LTR program conducts research using three different mechanisms:

Multi-Year Projects

These cost-shared projects between SC laboratories and private industry are performed in support of DOE missions but also are relevant to industry needs. LTR program funding to SC laboratories for these projects is typically from $100,000 to $250,000 per year for a three-year period. The industrial partner supports its research in at least an equivalent amount. Cooperative Research and Development Agreements (CRADAs) are used to implement these projects. CRADAs provide for protection of proprietary data and disposition of intellectual property. Projects that were initiated in Fiscal Year (FY) 1999 were chosen by an external peer review of proposals on the basis of scientific/technical merit and commercial potential. The reviewers were practicing experts in the subject area of the proposal, from at least three different institutions, who did not have a conflict of interest. Each reviewer provided comments on four evaluation criteria: scientific/technical quality, qualifications of key personnel and facilities, the work plan, and commercial potential. A fifth criterion on the industry partner commitment to the project (either funds-in or in-kind support) was evaluated by the DOE LTR program based on commitment letters from the industry partner. Proposals which received the strongest evaluations overall were chosen for funding.

.Each of the multi-year projects initiated in FY 1997 and 1998 was subjected to a mid-term review. The Principal Investigator gave a presentation on the project status to two independent experts in the project technical area. These interactive presentations were frequently attended by the industry partner researchers and management, and were overseen by the laboratory LTR manager and the DOE LTR management. Written evaluations were submitted by the reviewers to provide guidance to either continue the project as scheduled, suggest a revised workplan, or terminate the project. The reviews completed thus far have all been favorable. All of the multi-year projects which received FY 1999 funding from the LTR program (Total = $9.5 million) are included in this book of abstracts. The following ID codes for each abstract identify the national laboratory conducting the project: AL - Ames Laboratory, ANL - Argonne National Laboratory, BNL - Brookhaven National Laboratory, LBL - Lawrence Berkeley National Laboratory, ORL - Oak Ridge National Laboratory, PNL - Pacific Northwest National Laboratory, and SLAC - Stanford Linear Accelerator Center.

Rapid Access Projects (RAP)

These projects provide private industry, especially small businesses, with a means to solve difficult technical problems rapidly by tapping the unique expertise of SC laboratory scientists and engineers. These projects are implemented through a variety of flexible mechanisms, such as personnel exchanges, technical assistance to and consultations with small businesses, and small collaborative projects (CRADAs). Funding is allocated primarily on the basis of a merit review that emphasizes scientific/technical quality, commercial potential, and contribution to DOE's missions. These projects last from a few days to one year with LTR program funding to SC laboratories from $3,000 to $100,000 per project. Examples of each type of rapid access project are included in this book of abstracts. The total funding for rapid access projects was $1.8 million in FY 1999. A special request to the SC laboratories for RAP proposals, which were chosen for funding using external peer review, was used to allocate $0.55 million of these funds.

Major Industry Partnerships

Major industry partnership projects funded by the LTR program (Total = $2.7 million) are part of a large group of projects focused on one industrial segment. Abstracts of multi-year projects in support of the ACTI Partnership, which received FY 1999 funding from the LTR program, are listed as project sequence numbers 58 - 61. Abstracts of multi-year projects in support of the AMTEX Partnership, which received FY 1999 funding from the LTR program, are listed as project sequence numbers 62 - 66.

CONTACTS FOR THE LTR PROGRAM

U.S. Department of Energy

Dr. Walter M. Polansky, Director
Technology Research Division
Office of Advanced Scientific Computing Research

Dr. Samuel J. Barish, Team Leader
Laboratory Technology Research Program

Dr. Theodore Vojnovich
Dr. Bruce McNamara [*]
Ms. Sue Ellen Stottlemyer

Technology Research Division
U.S. Department of Energy, SC-32
19901 Germantown Road
Germantown, MD 20874-1290

Phone:	(301) 903-7485
Fax:	(301) 903-6067 (no more than 10 pages)
E-mail:	walt.polansky@science.doe.gov
	sam.barish@science.doe.gov
	ted.vojnovich@science.doe.gov
	bruce.mcnamara@science.doe.gov

Office of Science Laboratories

Ames Laboratory
Mr. Robert S. Harris, Manager
SC LTR Program
Ames Laboratory
Iowa State University
311 TASF
Ames, IA 50011
Phone: (515) 294-2635
Fax: (515) 294-3751
E-mail: harris@ameslab.gov

Argonne National Laboratory
Ms. Deborah Clayton, Manager
SC LTR Program
ITD-900
Argonne National Laboratory
9700 South Cass Avenue
Argonne, IL 60439
Phone: (630) 252-4694
Fax: (630) 252-5230
E-mail: dclayton@anl.gov

[*]On detail from Pacific Northwest National Laboratory

Brookhaven National Laboratory
Mr. Michael Furey, Manager
SC LTR Program
Brookhaven National Laboratory
P.O. Box 5000
Upton, NY 11973
Phone: (516) 344-2103
Fax: (516) 344-3729
E-mail: mfurey@bnl.gov

Fermi National Accelerator Laboratory
Dr. Bruce Chrisman, Manager
SC LTR Program
Fermi National Accelerator Laboratory
P.O. Box 500, MS 200
Batavia, IL 60510-0500
Phone: (630) 840-6657
Fax: (630) 840-4343
E-mail: chrisman@fnal.gov

Lawrence Berkeley National Laboratory
Mr. Chris Kniel, Manager
SC LTR Program
Lawrence Berkeley National Laboratory
Mailstop 90-1070
Berkeley, CA 94720
Phone: (510) 486-5566
Fax: (510) 486-6457
E-mail: crkniel@lbl.gov

Oak Ridge National Laboratory
Ms. Louise Dunlap, Director,
Partnerships Office
Phone: (423) 576-4221
E-mail: dunlaplb@ornl.gov
Oak Ridge National Laboratory
P.O. Box 5000
Oak Ridge, TN 37831

Dr. Terry Payne, Manager
SC LTR Program
Phone: (423) 574-0008
Fax: (423) 576-4181
E-mail: pay@ornl.gov

Pacific Northwest National Laboratory
Mr. Bruce Harrer, Manager
SC LTR Program
Pacific Northwest National Laboratory
P.O. Box 999, K9-21
Richland, WA 99352
Phone: (509) 375-6958
Fax: (509) 375-6838
E-mail: bj_harrer@pnl.gov

Princeton Plasma Physics Laboratory
Mr. Lewis D. Meixler, Manager
SC LTR Program
Office of Technology Transfer
Plasma Physics Laboratory
P. O. Box 451, M. S. 17
Princeton, NJ 08543
Phone: (609) 243-3009
Fax: (609) 243-2418
E-mail: lmeixler@pppl.gov

Stanford Linear Accelerator Center
Mr. Jim Simpson, Manager
SC LTR Program
Office of Technology Transfer
P.O Box 4349, MS 14B
Stanford, CA 94309
Phone: (650) 926-8604
Fax: (650) 926-4999
E-mail: jsimpson@slac.stanford.edu

Thomas Jefferson National Accelerator Facility
Dr. H. Frederick Dylla, Manager
SC LTR Program
Thomas Jefferson National Accelerator Facility
12000 Jefferson Avenue
Newport News, VA 23606
Phone: (757) 269-7450
Fax: (757) 269-6357
E-mail: dylla@jlab.org

ABSTRACTS OF MULTI-YEAR PROJECTS SUPPORTED IN FY 1999

ADVANCED MATERIALS

Design of Materials

1: *High Performance Tailored Materials for Levitation and Permanent Magnet Technologies*

ID:	ANL97-02	
PI:	George Crabtree Materials Science Division	
Phone:	630 252-5509	
Partner:	Superconductive Components, Inc. Columbus, OH	
FY 99 Funding:		$250K
Total Project Funds:		$750K

Background

Superconductivity has been actively pursued by scientists due to the ability of superconductive materials to conduct electrical currents without resistance, and hence to conserve energy. "High-temperature" superconductors (HTS), are hailed as a more viable technology because HTS metals lose resistance at temperatures well above the levels of ordinary superconducting metals, such as lead and aluminum. HTS materials are complex intermetallic compounds based on the oxide of copper:, e.g.. YBCO. As our understanding of the properties of HTS materials increases, applications, such as power transmission, superconducting magnets in generators, energy storage devices, particle accelerators, levitated vehicle transportation, rotating machinery, and magnetic separators, will become more practical. This project supports acceleration of superconducting technologies into US industry through DOE investments in basic research on advanced materials.

Research Objective

Argonne National Laboratory and Superconductive Components, Inc. are developing next-generation materials for levitation and trapped field magnet technologies. The focus of the project is to understand, and control the flux pinning mechanism which produces high critical current in the YBCO family of materials. Process variables, which require optimization to produce the maximum performance, will be evaluated, and techniques are being developed to fabricate complex shapes needed for specific applications.

Results

Basic materials research tools such as magnetization measurements (using SQUID: a vibrating sample magnetometer, and miniature Hall probes), magneto-optical imaging, and scanning electron microscopy are being used to reveal materials characteristics and processing conditions which lead to high performance. Key processing variables, that have been identified in the performance of the materials, include the high temperature growth rate, the post-growth low temperature oxygen anneal rate, and the rare earth composition of the starting materials. New processing techniques, which allow control of material performance at low and high magnetic field, are being developed.

Patent

1. B. W. Veal, H. Zheng, A. P. Paulikas, H. Claus, submitted 1999.

Publications

1. H. Zheng, M. Jiang, B. W. Veal, H. Claus, and B. Obst, *Physica C*, 301, 147 (1998).
2. H. Zheng, M. Jiang, Y. Huang, B. W. Veal, and H. Claus, *Physica,* C 307, 284-290 (1998).
3. H. Zheng, M. Jiang, R. Nikolova, V. Vlasko Vlasov, U. Welp, B. W. Veal, G. W. Crabtree and H. Claus, *Physica,* C, 309,17-24 (1998).
4. H. Zheng, M. Jiang, R. Nikolova, U. Welp, A. P. Paulikas, Yi Huang, G. W. Crabtree, B. W. Veal, and H. Claus, *Physica*, C, 1999, In Press.

2: *Ionically Conductive Membranes for Oxygen Separation*

ID:	LBL97-03	
PI:	Steven Visco	
Phone:	510-841-7242	
Partner:	Praxair, Inc. Tonawanda, NY	
FY99 Funding		$150K
Total Project Funds:		$475K

Background

The global market for industrial oxygen is estimated at $20 billion annually. The dominant technology for the production of commercial oxygen is cryogenic distillation. High capital equipment costs for cryogenic O_2 separation limits this technology to large installations. Accordingly, industrial suppliers of oxygen are developng technologies that can satisfy increasing demand for oxygen through smaller scale plants. One approach under development elsewhere is the use of mixed ionic-electronic ceramics. When such ceramic electrolytes are exposed to compressed air on one side and ambient pressure on the other, oxygen diffuses through the mixed conductor from the compressed side to the low-pressure side due to the chemical potential gradient of oxygen across the membrane. The drawback to scale-up of this technology is the need for a large compressor, which raises issues of compressor noise and reliability. Another problem is that permeation delivers ambient pressure oxygen. This project supports the DOE's investments in characterization of advanced materials and also in establishing efficient utilization of planetary resources.

Research Objective

Lawrence Berkeley National Laboratory and Praxair are developing a technology for efficient electrolytic extraction of oxygen from air. The project focuses on the use of high strength, ionic membranes, supported on porous, catalytic electrodes. Using this technology, high purity O_2 can be electrochemically pressurized as an integral part of the separation process.

The simplicity of operation of an electrolytic O_2 generator promises high reliability as well as low cost. Still, to survive as a commercial process, this approach must be cost-competitive to cryogenic production of O_2. Key to success is a low power consumption device combined with low fabrication costs. Power losses in the electrolytic oxygen cell will be related to ohmic losses across the electrolyte membrane, charge transfer polarization at the electrode/electrolyte interfaces, and mass transfer polarization across the electrodes.

Results

The LNBL team was scheduled to fabricate a planar oxygen separation membrane, test the device, and deliver several planar oxygen pumps to Praxair. The oxygen separation devices were tested and their performance met or exceeded target goals. Current work focuses on characterization and processing of films to achieve optimal porosity and their layering onto porous electrode substrates. It has been found that interfacial reactions effect oxygen pumping performance.

Invention Disclosures

1. Improved Electrode-Electrolyte Structure for Solid State Electrochemical Devices, S-90,387.
2. Alloy Support Structure for Ceramic Electrode Devices.
3. Surface Additives for Enhanced Electrode Performance, S-90, 388.

3: ***Light Emission Processes and Dopants in Solid State Light Sources***

ID:	LBL97-13
PI:	Eugene Haller Material Sciences Division
Phone:	510 486-5294
Partner:	Hewlett-Packard Company Palo Alto, CA
FY99 Funding:	$250K
Total Project Funds:	$750K

Background

Light emitting diodes (LEDs) functioning in the red and infrared have been manufactured in large quantities since the 1960s. However, until very recently, only very inefficient and dim LEDs were available in the green and, especially, in the blue. Although there are a handful of semiconducting materials with sufficiently wide bandgaps to function in principle in the blue region of the spectrum, fundamental material properties and limitations have prevented bright and efficient diodes from being made. Recently, breakthroughs in the heteroepitaxial growth of gallium nitride (GaN) and its alloys with indium and aluminum have changed the blue and green LED technology outlook. Formerly, it was believed that III-V nitride layers had too high a defect density to function as LEDs. Nevertheless, a Japanese company (Nichia) has developed a family of blue and green LEDs based on GaN that are bright and efficient. For the last three years, Japanese companies have been manufacturing and selling blue GaN LEDs in bulk quantities.

Research Objective

Lawrence Berkeley National Laboratory and Hewlett-Packard, the leading producer of LEDs, are investigating the fundamental light-emitting mechanism of blue and green LEDs. Hewlett-Packard is providing GaN and InGaN structures grown with their metal-organic chemical vapor deposition equipment. Research is being performed in four technical areas: (1) Doping related strain effects in GaN and InGaN epitaxial layers, (2) Metal/GaN contacts, (3) Localization properties of dopants and defects, and (4) Carrier transport in layers and devices.

Results

In the first technical area, work performed with multilayer structures was used to show that compressive film stress and Si concentration, which were found to be positively correlated in previous work, could be varied independently by appropriate changes in growth conditions. This is of considerable importance to Hewlett-Packard, because reliable production of thick GaN layers had been limited by cracking induced by the Si dopant. In the metal contacts technical area, a new method for obtaining ohmic contacts based on manipulating the bandgap via the formation of “localized” energy levels has been developed and is being tested in GaN. In work related to the localization and transport topics, optical measurements have been performed in diamond anvil cells with p-doped GaN single crystals, GaN, AlGaN, and InGaN single layers, and GaN/InGaN multilayer structures. These results are being used to understand the mechanism of light production in III-V nitrides. The program advances the DOE’s Office of Basic Energy Science mission in synthesis and characterization of advanced materials.

Award

1. James C. McGroody Award

Publications

1. W. Shan, W. Walukiewicz, E. E. Haller, B. D. Little, J. J. Song, Z. C. Feng, M. Shurman and R. A. Stall, *J. Appl. Phys.* 84(8), 4452 (1998).
2. W. Shan, J. W. Ager III, W. Walukiewicz, E. E. Haller, B. D. Little, J. J. Song, Z. C. Feng, M. Shurman and R. A. Stall and B. Goldenberg, *Appl. Phys. Lett.* 72(18), 2274 (1998).
4. W. Shan, J. W. Ager III, W. Walukiewicz, E. E. Haller, B. D. Little, J. J. Song, B. Goldenberg, Z. C. Feng, M. Schurman, and R., A. *Stall, Mat. Res. Soc.Proc.* Vol. 499, 36 (1998).
5. W. Shan, J. W. Ager III, K. M. Yu, W. Walukiewicz, E. E. Haller, M. C. Martin, W. R. McKinney and W. Yang, *J. Appl. Phys.* 85(12), 8505 (1999).
6. L. T. Romano, C. G. Van de Walle, R. Lau, J. W. Ager III, W. Götz, and R. S., Kern, *Physica B*, in press.

4: *Combinatorial Discovery and Optimization of Novel Materials for Advanced Electro-Optical Devices*

ID: LBL97-18
Partner: Xiao-Dong Xiang
Materials Science Division
Phone: 510 486-4864
NZ Applied Technologies
Woburn, MA
FY99 Funding: $250K
Total Project Funds: $750K

Background

Advanced materials are one of the critical building blocks of emerging photonic technology, which is the foundation for a new industrial base. Complex oxide ceramics (ternary and higher order compounds) exhibit a wide range of technologically significant properties such as the electro-optic effect. The rapid expansion in the types of phenomena exhibited by modern advanced ceramics has revived interest in the use of complex oxides for advanced optical device applications. However, due to the complexity of multi-component oxides, searching for new materials or optimization of existing materials is a forbidding task for the materials community.

Research Objective

Lawrence Berkeley National Laboratory in collaboration with NZ Applied Technologies are developing thin film, complex oxide ceramics used for the fabrication of electro-optical devices. The objective of the project is to use combinatorial synthesis and screening to first evaluate a wide range of oxide materials and compounds, and optimize advanced oxide materials for electro-optical devices. Subsequently, heteroepitaxial thin film growth methods, developed at NZAT, will be used to fabricate electro-optical devices based on the search and optimization results.

Results

The work has developed combinatorial materials synthesis and high throughput screening techniques to accelerate the speed of materials research. Thin film materials libraries containing thousands of different compositions or continuous ternary phase diagrams with epitaxial quality can be routinely fabricated.

High throughput screening techniques for evaluating electro-optical effect of materials libraries have also been developed. Rutherford backscattering and x-ray diffraction studies are being used to observe growth processes and crystalline formation of thin films. Overall, the method of stepwise film synthesis from precursor multilayers has been shown to yield device quality films, comparable to conventional synthesis methods. Additionally, the new films are being examined with a novel optical system, developed for sensitive electro-optical measurements. The project supports the DOE's investments in characterization of structure and functionality of advanced materials.

Award

1. 1996 Discover Magazine Award for Technological Innovation.

Patents

1. "Advanced Phosphors" US patent application #09/016,577.
2. "Low Loss Composition of $(Ba_xSr_yCa_{1-x-y})TiO_3$", US patent , pending

Publications

1. X.-D. Xiang, *Annual Review of Materials Science* 29, (1998).
2. X.-D.Xiang, *Materials Today* 1, 23, (1998).
3. E. D. Issacs, M. Kao, G.Aeppli, X.-D.Xiang, X.Sun, P. Schultz, M.A.Marcus, G. S.Cargill, R.Haushalter, *Appl. Phys. Lett*. 73, 1820 (1998).
4. I. Takeuchi, H. Chang, C. Gao, P. G. Schultz, and X.-D. Xiang, R. P. Sharma, M. J. Downes, and T. Venkatesan, *Appl. Phys. Lett*. 73, 894 (1998).
5. H. Chang, I. Takeuchi, and X.-D. Xiang, *Appl. Phys. Lett*. 74, 1165 (1999).
6. H. Chang, C. Gao, I Takeuchi, Y. Yoo, J. Wang, P. G. Schultz, and X.-D. Xiang, R. P. Sharma, M. Downes, and T. Venkatesan, *Appl. Phys. Lett*. 72, 2185 (1998).
7. Jingsong Wang, Young Yoo, Chen Gao, Ichiro Takeuchi Xiaodong Sun, X-D. Xiang, Peter G. Schultz, *Science* 279, 1712 (1998).
8. Xiao-Dong Sun and X.-D. Xiang, *Appl. Phys. Lett*. 72, 525 (1998).

Seven more articles related to this project have been published in peer reviewed journals.

5: *Interplay Between Interfacial Properties and Dielectric and Ferroelectric Behaviors of Barium Strontium Titanate Thin Films*

ID:	PNL99-08	
PI:	Yong Liang Environmental Molecular Sciences Laboratory	
Phone:	509 376-8565	
Partner:	Phoenix Corporate Research Laboratories Motorola, Inc. Tempe, AZ	
FY99 Funding:		\$125K
Total Project Funds:		\$750K

Background

Barium strontium titanate (BST) and related materials are entering commercial use for integrated circuit manufacture as conventional materials reach their fundamental limits. BST films have capacitance, leakage, and related electrical properties that surpass integrated circuit device requirements. One of the most important steps towards understanding the interplay between interfacial properties and dielectric and ferroelectric behaviors of BST ($Ba_{1-x}Sr_xTiO_3$) is the growth of high quality BST films on Si substrates. Successful epitaxial growth of crystalline BST on Si(001) is thought to require the formation of a two-dimensional interfacial silicide layer involving either Ba or Sr as the initial step. Bulk thermodynamics suggests that this thin silicide layer is required to stabilize the interface.

Research Objective

This collaboration between Pacific Northwest National Laboratory and Motorola is designed to gain a fundamental understanding of how interfaces affect the dielectric and ferroelectric properties of BST thin films, and to use such knowledge to improve the design and processing of BST thin film-based devices.

The goal of the project is to address two specific issues of significant concern in BST thin-film technology: (1) the effect of interfacial chemistry and stress on the dielectric and ferroelectric properties of BST thin films, and (2) ferroelectric behavior at the nano-scale level.

Results

PNNL is working to prepare, isolate, and characterize an ultrathin silicide layer using Sr as the alkaline earth metal. Si(001)-(2x1) surfaces were prepared in ultra high vacuum (UHV) by rapid desorption of the native oxide layer. These surfaces were exposed to Sr from an effusion cell in an oxide MBE chamber as a function of evaporation rate, substrate temperature, and total dose. The resulting interfaces were characterized during growth with reflection high-energy electron diffraction (RHEED), and after growth with low-energy electron diffraction (LEED), x-ray photoemission (XPS), and x-ray photoelectron diffraction (XPD). Additionally, the team is initiating STM investigations to further elucidate this interface structure. Motorola has focused on developing an MBE process for depositing epitaxial $SrTiO_3$ on silicon, and has conducted numerous experiments to optimize the interface between $SrTiO_3$ and silicon. Physical and electrical testing of these structures have been performed to determine interface roughness, interface layer formation, interface state density, dielectric properties (permittivity, leakage, etc.), and stability vs. post-growth processing. PNNL is currently integrating the $SrTiO_3$ film into a metal-oxide-semiconductor transistor structure. This project supports DOE's commitment to basic energy sciences in fostering the synthesis, processing, and characterization of advanced materials.

6: *An Advanced Hard Carbon Plasma Deposition System with Application to the Magnetic Storage Industry*

ID: LBL98-16
PI: Andre Anders
Accelerator and Fusion Division
Phone: 510 486-6745
Partner: CSC-Commonwealth Scientific Corporation
Alexandria, VA

FY99 Funding: $175K
Total Project Funds: $750K

Background

Diamond coatings have a number of properties, such as hardness and chemical inertness, which make them attractive for use in magnetic storage applications. The use of these coatings on computer hard disks and read/write heads is limited, however, due to difficulties associated with deposition of particulate free films. For this particular application, difficulties associated with film deposition are aggravated by the small "fly distance" of the read head surface from the hard disk surface, commonly about 10-20 nm. This implies that coatings on both surfaces be deposited, devoid of any particulate material or defect. An additional requirement is that the deposition thickness on both surfaces be minimized, perhaps to as low as 5 nm, and that the film be continuous. Film deposition by pulsed, filtered, cathodic-arc plasma-generation has been identified as a promising candidate for these process requirements.

Research Objective

Lawrence Berkeley National Laboratory and CVC Commonwealth Scientific Corporation (CSC) are combining resources to develop next-generation, industrial scale, filtered arc plasma deposition equipment. The objective of the project is to use the plasma deposition system to coat computer hard disks and read/write heads with ultra-thin diamond-like carbon films. CSC intends to couple the plasma source and macro-particle filter to complete macro-particle suppression; improve plasma transmission (hopefully double the rate compared to present efforts); trap macro-particles within the filter; and design a compact system that can be directly plugged into existing sputter coating facilities. The project extends the DOE's research in advanced materials, and synthesis and processing by ions and plasmas to market application.

Results

A plasma source has been developed and tested for deposition of ultra thin films. The source has been operated with arc pulses of up to 2000 A, 500 µs duration, with a pulse repetition rate of 10 Hz. These parameters are a close match to the requirements of a viable industrial deposition source. The filter efficiency has performed above expectations because of its compact design length of 10 cm. The power supply is also compact and is matched to the power requirements of the source and filter. The successful demonstration of the deposition system represents a breakthrough in coatings technology for carbon deposition on hard disks.

Publications

1. M. M. M. Bilek and A. Anders, *Plasma Sources Science & Technology,*Vol. 8, 488-493 (1999).
2. A. Anders, Invited Talk at the International Conference on Metallurgical Coatings and Thin Films, San Diego, April 1999, *Surface and Coatings Technology,* accepted 1999.
3. A. Anders, R.A. MacGill, and T. A. McVeigh, *Review of Scientific Instruments,* accepted 1999.

Patents

1. Patent Application, filed on March 31, 1999, "triggerless" arc initiation, and new plasma "twist" filter and plasma source design.
2. Patent disclosure describing method and apparatus of plasma injection into a plasma homogenizer, August 1999.

7: *A Facility for Studying Micromagnetic Structures*

ID:	LBL95-12	
PI:	Howard Padmore	
Phone:	510 642-5787	
Partner:	IBM San Jose, CA	
FY99 Funding:		$94K
Total Project Funds:		$900K

Background

During the 1990s, the data density attainable by magnetic recording technology increased at a rate of 60 percent a year, just as predicted by Moore's Law of transistor density. As miniaturization of devices advances to the point where the behavior of small numbers of atoms deviates from that of the bulk sample, techniques to explore nanometer scale volumes of materials surfaces become imperative.

Research Objective

The goal of this project between Lawrence Berkeley National Laboratory and IBM is to produce a powerful and unique tool for microscopic imaging of magnetic materials and to use this tool to develop new magnetic materials for high-density information storage. The microscope is based on a full-field photoelectron emission technique, and magnetic information is extracted using a synchrotron radiation spectroscopy known as X-ray Magnetic Circular Dichroism (X MCD). The microscope will have elemental and chemical selectivity, combined with surface sensitivity, and the ability to measure surface magnetic moments. This combination of features is unique in the array of tools currently used to study magnetic materials. The project supports DOE's mission in basic sciences for the study of advanced materials.

Results

The project's initial work on the PEEM1 microscope has achieved the theoretical best resolution of 20 nm. This sets the new world standard for any type of soft x-ray microscopy. It has also been demonstrated that linear dichroism can be used to image antiferromagnetic domains.

The ability of linear dichroism in x-ray absorption spectroscopy to measure antiferromagnetic moments is a unique aspect of this work and has opened up a tremendous range of studies. The antiferromagnetic structure of NiO surfaces has recently been studied, and a significantly reduced anti-ferromagnetic ordering temperature (Neel temperature), in the region of line defects, has been measured. This work has been extended to observe clear domain structure in anti-ferromagnetic $LaFeO_3$, and a reduced Neel temperature in comparison to the bulk has been measured. Systems where a thin ferromagnetic layer is deposited on the antiferromagnetic substrate are now being studied. In the case of Co on $LaFeO_3$, the ferromagnetic domains are differentiated, using circular dichroism, from the antiferromagnetic substrate, using linear dichroism, and the direct coupling between the two can be observed. Coupled systems of antiferromagnetic-ferromagnetic layers are the basis of many devices for the control and manipulation of electron spin, for example in spin valves used in magnetic memory. This is the first microscopy that can study this fundamental magnetic coupling phenomenon, and will clearly have tremendous impact in basic science and technology.

Publications

1. J. Stohr, H. A. Padmore, S. Anders, T. Stammler and M. R. Scheinfein, *Surface Review and Letters*, Vol. 5, No. 6 (1998).
2. J. Stohr, A. Scholl, T. Regan, S. Anders, J. Luning, M. R. Scheinfein, H. A. Padmore and R. L. White, *Phys. Rev. Lett*., 83(9), 1862 (1999).
3. A. Scholl, J. Stohr, J. Luning, J.-P. Locquet, J. Fompeyrine, J. W. Seo, H. Siegwart, F. Nolting, S. Anders, E. Fullerton, M. R. Scheinfein and H. A. Padmore, *Science*, submitted Aug. 1999.

8: *Critical Vacancy-Driven Phenomena in High-Energy Ion-Implanted Silicon*

ID:	ORL 98-18	
PI:	Tony Haynes	
Phone:	423 576-2858	
Partner:	Lucent Technologies Murray Hill, NJ	
FY99 Funding:		$177K
Total Project Funds:		$750K

Background

Ion implantation is a technique to introduce in a controlled manner an element into a material or thin film. High-energy (MeV) ion implantation is now being rapidly introduced into integrated circuit manufacturing because it provides process simplification and improved materials performance. However, the technique introduces an imbalance of excess vacancies and vacancy-cluster defects in the near-surface region of a silicon crystal, which can cause problems during subsequent processing.

Research Objective

Teaming Oak Ridge National Laboratory with Bell Labs and Brookhaven National Laboratory provides access to a suite of new, complementary capabilities for experiment and modeling that promise to elucidate vacancy behavior. The objective of this project is to develop sufficient understanding of the physical mechanisms underlying the evolution of these defects and interactions with dopant atoms to enable accurate prediction and control of dopant diffusion and defect configurations during processing. The project will develop a systematic method to generate large, controllable, and spatially-isolated vacancy concentrations in silicon using high-energy implantation.

Results

The evolution of vacancy profiles during thermal treatments, monitored by conventional techniques such as positron annihilation spectroscopy, as well as some new methods, have recently been developed by the team. For instance, two new methods have been demonstrated for measuring the depth profiles of defects produced by high-energy implantation: (1) measurement of x-ray diffuse scattering cross-section profiles using a submicron x-ray beam at the Advanced Photon Source, and (2) measurement of vacancy cluster depth-profiles by labeling the clusters with gold atoms. Experimental results from this project are also being modeled using new computer simulation tools developed at Bell Labs. This project benefits the telecommunications and microelectronics industries, and contributes to improvements in cost and performance for a wide range of high-tech products, from computers and cellular phones to digital television. It supports the DOE programs in materials sciences and extends ongoing ion-solid physics and x-ray scattering at ORNL into new areas. The project will also strengthen the national capability for advanced processing of electronic materials—an enabling technology for DOE programs in energy conversion, and defense.

Publications

1. V. C. Venezia, D. J. Eaglesham, T. E. Haynes, A. Agarwal, D. C. Jacobson, H.-J. Gossmann, and F. H. Baumann, *Appl. Phys. Lett.*, 73, 2980 (1998).
2. V. C. Venezia, T. E. Haynes, A. Agarwal, H.-J. Gossmann, L. Pelaz, D. C. Jacobson, D. J. Eaglesham, and J. L. Dugganpp, *Proc. 15th Int'l Conf. on Applic. Of Accelerators in Research and Industry*, 784–788 (1999).
3. V. C. Venezia, T. E. Haynes, A. Agarwal, L. Pelaz, H.-J. Gossmann, D. C. Jacobson, and D. J. Eaglesham, *App. Phys. Lett.*, 74, 1299 (1999).
4. M. Yoon, B. C. Larson, J. Z. Tischler, T. E. Haynes, J. S. Chung, G. E. Ice, and P. Zschack, *Applied Physics Letters*, accepted 1999.

9: *Improved Materials for Semiconductor Devices*

ID:	PNL98-17	
PI:	Suresh Baskaran	
	Materials Sciences Department	
Phone:	509 375-6483	
Partner:	SEMATECH	
	Austin, TX	
FY99 Funding:		$250K
Total Project Funds:		$750K

Background

The increasingly higher performance required of semiconductor devices has resulted in a need for new materials to reduce the capacitance between metal conductor lines (interconnects) on semiconductors. The ability of a material to reduce capacitance losses is defined by its dielectric constant, and the development of interlevel dielectric materials with much lower dielectric constants (k<<4) than what is currently available is the focus of considerable attention within the semiconductor industry. In addition to improving electrical performance (power consumption, signal speed, and propagation noise), such materials could potentially offer significant reductions of about $500 million annually in fabrication costs for semiconductors.

Research Objective

Pacific Northwest Laboratory and Sematech are developing mesoporous silica dielectric films for application in semiconductor interconnects. PNNL's focus is the design and synthesis of novel surfactant-templated porous films, including pore design, characterization, surface modification and initial process development. SEMATECH is responsible for characterization of film performance, and evaluation in relation to interconnect processing for semiconductors.

Results

The surfactant and deposition solution chemistry have been investigated for the synthesis of porous films. Pore surface chemistry was modified through a series of dehydroxylation treatments to obtain low, stable values of dielectric constant. Dielectric constants less than 2.5 were obtained on films prepared with a cationic cetyl trimethyl ammonium chloride surfactant. Highly porous films with low dielectric constants (<2.2), high thickness uniformity, and low surface roughness were demonstrated on 4-inch wafers using non-ionic polyoxyethylene ether surfactants. Using nuclear reaction analysis and the Rutherford backcattering facility at the Environmental and Molecular Sciences Laboratory at PNNL, porosity in the surfactant-templated films was determined to be 50-60%. The elastic modulus measured by picoindentation indicates that the films should have adequate mechanical integrity for multilevel integration, including the ability to withstand stresses from chemical mechanical polishing over a dense silica cap layer. Future research will include surfactant design and porosity control to obtain lower dielectric constants, investigation of surfactant-compatible additives to tailor pore size and porosity, and continuous process and nanostructure modifications based on process and film evaluations at SEMATECH. The project continues the DOE's commitment to improved materials design and characterization.

Publications

1. S. Baskaran, J. Liu, K. Domansky, X. Li, N. Kohler, G. Fryxell, S. Thevuthasan, L. Q. Wang, R. E. Williford, *App. Phy. Letts.*, submitted 1999.
2. K. Domansky, J. Liu, L Q. Wang, M. Englehard, S. Baskaran, *App. Phy. Letts*., submitted 1999.

10: *Photocatalytic Metal Deposition for Nanolithography*

ID:	ANL99-13	
PI:	Tijana Rajh Chemistry Division 630 252-3542	
Partner:	Hewlett Packard Research Laboratories Palo Alto, CA	
FY99 Funding:		$125K
Total Project Funds:		$750K

Background

A major technical impediment for the development of mesoscopic scale electronic devices is obtaining molecular scale conducting patterns. Based on the parameters that are optimized in highly efficient photochemical energy conversion in natural photosynthesis, Argonne National Laboratory has developed a new mask-less photoelectrochemical method for depositing conductive metal patterns with nanometer scale precision. This technology will enable the rapid prototyping and manufacturing of mesoscopic electronics and offers the potential of low-cost small batch manufacturing and unparalleled levels of electronic integration.

Research Objective

ANL and Hewlett Packard will utilize this new technology to fabricate miniaturized (ultimate resolution limit of 1 nm) and rugged electrical interconnects and biomolecular electronic devices on any surface or in solution. This project will enable the 3-D integration of passive and active components of mesoscopic integrated conformal electronics.

In addition, this technology provides a unique advantage compared to other electronic technologies, because the semiconductor substrate (precursor) can also perform active function in the bioelectronic device. Conductor precursors, semiconductor metal oxide nanoparticles modified with chelating agents, that bind metal cations (copper, silver, and gold), will be synthesized. Biological templates will be used to self-assemble conductor precursors in order to achieve spacial resolution via photocatalysis. The fast photoresponse of semiconductor nanodots also provides high time resolution. Based on a fundamental understanding of electron transfer reactions in this biomimetic approach, precursor formulations will be developed and characterized for photoelectrochemical response, redox stability, and mechanical properties. Precursors will be deposited on a range of substrates (silicon, glass, plastic, metals, ceramics, etc.) or in solution. Conductive patterns formed by catalytic semiconductor assisted solid state deposition of copper, silver, or gold will be studied as a function of nanoparticle size, reduction technique, and nanoparticle-chelate association complex. Interconnects and biomolecular assemblies will be studied to ascertain morphology, function, and 3-D characterization as a function of processing methodology. The technology developed in this project is an extension of DOE's efforts to promote characterization of materials useful to nanotechnology.

11: *Smooth Diamond Films for Friction and Wear Applications and Chemically Protective Coatings*

ID:	ANL97-05
PI:	Alan Krauss
Phone:	630 252-3520
Partners:	Flowserve Corporation Kalamazoo, MI Applied Science and Technology (ASTeX) Woburn, MA
FY99 Funding:	$ 250K
Total Project Funds:	$ 750K

Background

Diamond has a number of properties which, in principle, make it an exceptional material for a large number of applications. In particular, the extreme hardness, chemical inertness, and low coefficient of friction (comparable with that of Teflon™) make it an ideal candidate for a wide range of applications involving sliding or rolling contact between moving surfaces. However, conventional diamond chemical vapor deposition (CVD) methods produce coatings with extremely rough surfaces. This roughness has limited the development of diamond film technology for tribological applications, and penetration of diamond film technology into these markets has been disappointingly slow.

Research Objective

Argonne National Laboratory and Flowserve have adapted a process for the production of diamond coatings that are 10-100 times smoother than those produced by existing processes. The focus application of the project is end face mechanical seals, which are used to prevent the leakage of gases and liquids in equipment with rotating shafts. The benefits obtained in terms of energy savings, increased productivity, reduced maintenance, and reduced release of environmentally hazardous materials for this single application will be substantial.

Results

ANL has developed a process for the deposition of ultrasmooth diamond coatings on surfaces. Films produced by this process have been shown to possess tribological properties which eliminate the problems which have so far limited the use of diamond coatings for applications involving moving parts. 3 µm, 6 µm, and 30 µm thicknesses of nanocrystalline diamond have been deposited on silicon carbide seal rings. The seals have been tested up to 150 psi for eight hours. The diamond coated seals were examined by SEM and showed no sign of wear. The technology developed will also be directed to applications in manufacturing and transportation and will continue the DOE's advancement of environmentally safe technologies in the private sector.

Publications

1. A. Erdemir, C. Bindel, G. R. Fenske, C. Zuiker, R. Csencsits, A.R. Krauss, D.M. Gruen, *Diamond and Related Mater*., 5, 923 (1996).
2. A. Erdemir, M. Halter, G. R. Fenske, C. Zuiker, A. R. Krauss, D. M. Gruen, *Tribology Trans*., 40, 667 (1997).
3. A. Erdemir, M. Halter, G. R. Fenske, A. R. Krauss, S. M. Pimenov, V. I. Konov, *Surf. Coat. Technol*., 94, 537 (1997).

Patents

1. Fullerenes as precursors for diamond film growth.
2. Improved method for the preparation of nanocrystalline diamond thin films.

Patents Pending

1. A method for improving the field emission characteristics of diamond thin films.
2. Diamond field emission thin film coatings on discrete field emitter arrays.
3. Smooth diamond films as low friction, long-wear surfaces.

12: *Near-Frictionless Carbon Coatings*

ID:	ANL98-03
PI:	Ali Erdemir Energy Technology Division
Phone:	630 252-6571
Partners:	Front Edge Technology Baldwin Park, CA Diesel Technology Company Kentwood, MI Stirling Thermal Motors, Inc. Ann Arbor, MI
FY99 Funding:	$250K
Total Project Funds:	$750K

Background

Friction-reducing coatings are often applied to moving parts of precision mechanisms that use sliding, rolling, or rotating devices. However, applying such coatings may be difficult, time-consuming, or impossible on substrate materials such as plastics, ceramics, and certain metal alloys. Coating durability can also be a problem.

Research Objective

Argonne National Laboratory is working with their industry partners to optimize the growth conditions and tribological performance of a near-frictionless carbon film (NFC) and will transfer this technology for use in components in diesel engines. The project forwards the DOE's interest in technologies which increase energy efficiency and component reliability.

Results

Ultra-low-friction, or near-frictionless, carbon film coatings that can be deposited at low temperature on virtually any substrate and are exceptionally wear-resistant and durable on steel, ceramics, and plastics, have been developed. Research to date has shown that the NFC films have the potential to overcome many of the friction and wear problems experienced by critical engine components, such as fuel injectors operating in sulfur-free diesel and gasoline fuels and swash plates operating under extreme contact pressures.

The film has exceptional wear resistance and durability with a coefficient of friction 0.001 when measured in a dry nitrogen atmosphere. The deposition process has been optimized to produce coatings on ceramic and metallic substrates at low temperatures to avoid risking damage to heat-sensitive materials. Fuel lubricity tests in a specially designed friction and wear test machine indicated that NFC coatings were compatible with ethanol and sulfur- free diesel fuels and provided dramatically improved friction and wear performance. Coatings with lower or no hydrogen seem to work better in ethanol environments, while in diesel fuels and under dry or marginally-lubricated conditions hydrogenated films worked the best. These findings have led to the conclusion that films have to be tailored or formulated for a specific application. Fundamental studies have focused on model hydrogen-saturated carbon compounds using quantum mechanical methods. Specifically, theoretical energies and vibrational spectra (IR and Raman frequencies) have been calculated and currently being compared with experimental results. Future fundamental research will explore the critical link between film microstructure chemistry and ultralow friction nature of the NFC films. Applied research will focus on testing of optimized coatings under conditions prototypical of actual engine applications.

Awards 1998

1. 1998 R&D 100 Award.
2. Bisson Award, Society of Tribologists and Lubrication Engineers
3. ANL, Director's Special Award, Pacesetter Award
4. ASME, Innovative Research Award

Patents

1. Pending patent: Method to produce ultralow friction carbon films.

Publications

1. A. Erdemir, G. R. Fenske, J. Terry, P. Wilbur, *Surface and Coatings Technology*, 94 (1997).

13: ***Development of Bismuth-Based Superconducting Wire with Improved Current Carrying and Flux Pinning Properties***

ID:	ANL99-15	
PI:	Victor Maroni Chemical Technology Division	
Phone:	630 252-4547	
Partner:	American Superconductor Westborough, MA	
FY 1998 Funding:		$125K
Total Project Funds:		$750K

Background

Progress in the commercialization of electric power equipment fabricated with high temperature superconducting materials has been limited by performance issues associated with the maximum achievable engineering critical current density, J_e, in long- length composite conductor. One of the most advanced conductors available today for such applications is the silver-clad $(Bi,Pb)_2Sr_2Ca_2Cu_3O_y$ (called Ag/Bi-2223) composite in multifilament form. However, the J_e of Ag/Bi-2223 at 77 K in magnetic fields of 1 Tesla or more is not presently adequate for most types of motors, generators, transformers, current limiters, and related power system components.

Research Objective

Argonne National Laboratory and American Superconductor are conducting research aimed at investigating two new pathways to fabricate the next generation of improved bismuth-based superconducting wire. The project extends DOE commitments in characterization and design of advanced materials for the acceleration of superconducting technologies to US markets.

One pathway is focused on the controlled growth of strong flux pinning centers in Ag/Bi-2223 filaments by the implementation of special heat treatment procedures. These create a transient thermodynamic state that promotes the growth of selected second phase nanocrystallites having the correct size, shape, and spatial distribution to induce strong inter- and intra-granular flux pinning. The second pathway involves reducing the **c-**axis blocking layer gap (between CuO_2 planes) in layered bismuth cuprates by demonstrating fabrication of the silver-clad $(Bi,Pb,Cd)_1Sr_2Ca_1Cu_2O$ (M-1212) along lines that have been developed for Ag/Bi-2223. The "in-principle" advantage of M-1212 over Bi-2223 stems from the shorter (by ~ 4 D) blocking gap in M-1212 due to fewer atomic layers in the **c-**axis repeat unit. From preliminary work, there are existing laboratory scale indications that both pathways can lead to significant improvement in the performance of bismuth-based high temperature composite conductors.

14: *Development of Buffer Layers Suitable for Deposition of Thick Superconducting $YBa_2Cu_3O_7$ Layers by a Post-deposition Reaction Process*

ID:	BNL98-05
PI:	Masaki Suenaga Department of Applied Science
Phone:	516 344-3518
Partner:	Oxford Superconducting Technology Carteret, NJ
FY99 Funding:	$250K
Total Project Funds:	$750K

Background

A principal advantage of using high-temperature superconducting (HTS) ceramics in the construction of a high field electromagnet is that ceramics exhibit their superconducting state at easily accessible cryogenic temperatures. Unfortunately, these ceramics possess a crystallographic anisotropy that makes them highly susceptible to magnetic fields oriented parallel to the crystallographic c-axis of the ceramic. This feature of ceramic films has been a barrier to the use of ceramics in HTS applications.

Research Objective

Brookhaven National Laboratory and Oxford Superconducting Technology are developing superconductive tapes by deposition of thick $YBa_2Cu_3O_7$ on a metallic substrate, e.g., textured Ni. The use of textured nickel as a substrate provides a route to axial alignment of the HTS ceramic. The objectives of the project are to examine the compatibility of some of the known candidate buffer $YBa_2Cu_3O_7$ layers, deposited by the post-deposition reaction process, and to seek other buffer candidate materials.

Results

The studies to date on the formation of thick (> 3 mm) $YBa_2Cu_3O_7$ layers on CeO_2 identified the formation of an interfacial phase by the chemical reaction between $YBa_2Cu_3O_7$ and CeO_2. This reaction tends to make the growth of c-axis oriented $YBa_2Cu_3O_7$ difficult. However, a ~ 5 mm thick $YBa_2Cu_3O_7$ layer on bi-axially textured Ni tape (~ 3 mm wide), using $CeO_2/ZrO_2/CeO_2/Ni$ as an epitaxial template and a diffusion barrier, has been grown. This tape carried a critical current density J_c = 0.5 MA/cm^2. Although this J_c result is encouraging, further improvement in the values of J_c may be difficult due to the interfacial chemistry. Accordingly, at Oxford Superconducting, experimental buffer layer architectures on the textured Ni tapes as well as on single crystalline oxide substrates are being fabricated using pulsed laser deposition. These will be tested at BNL for compatibility with the Ba_2F processed $YBa_2Cu_3O_7$. While the materials selection process for the buffer layer is proceeding, a new dedicated vacuum chamber for buffer layer deposition is being constructed. Also, the current electron beam evaporation chamber is being modified such that $YBa_2Cu_3O_7$ precursor layers can be deposited on a long length (~300 mm) substrate to investigate heat treating methods for long tapes. If the project is successful, it will be possible to fabricate long lengths of the conductors which are suitable for applications in electrical power devices and very high magnetic field magnets. Identification of materials and process technologies which will accelerate introduction of HTS devices to US industry is compliant with DOE superconductivity initiatives.

15: *Nanometer Characterization and Design of Molecular Lubrication for the Head-Disk Interface*

ID:	LBL98-10
PI:	Miquel Salmeron
Phone:	510 642-6704
Partner:	Seagate Technology, Inc. Fremont, CA
FY99 Funding:	$153K
Total Project Funds	$465K

Background

Information recording density in magnetic storage (hard disks) is currently increasing at an annual rate greater than 60%. In the quest for ever higher performance, the trend in the industry is toward even smaller head to disk spacing. The read head of a hard disk rotates within 10 nanometers of the disk surface. This surface is protected from damage during accidental contacts by an approximately 2 nanometer thick lubricating film. Liquids exhibit unique physical properties when confined between surfaces separated by molecular dimensions and when spread in films of molecular scale thickness. Although current film thickness is now less than the length of one lubricant molecule, industry standard characterization methods, based on optical techniques, are limited to micron-scale lateral resolution.

Research Objective

Lawrence Berkeley National Laboratory and Seagate Technology are designing molecular lubrication for the head-disk interface (HDI). The goal of the project is to characterize and design advanced lubricants with properties tailored for the next generation of magnetic storage devices.

Results

LBNL has developed a scanning polarization-force microscopy technique, which is the first non-invasive technique capable of imaging the structure of liquid films with approximately 50 nanometer lateral resolution and sub-nanometer normal resolution. This unique characterization method is being used to correlate nanoscale structure and properties with microscale engineering measurements and to develop and verify the performance of optimized, tailored HDI lubricants. Exploratory studies on advanced lubricant-overcoat systems are being carried out to identify critical performance parameters, with the final goal of designing an HDI lubricant with optimized wetting and spreading properties, tailored for future generations of ultra-high density storage devices. The project supports DOE's investments in the basic sciences to investigate the atomistic basis of materials behavior.

Publications

1. L. Xu, D.F. Ogletree, M. Salmeron, H. Tang, J. Gui and B. Marchon., *J. Chem. Phys.*, Submitted 1999.

16: *Interfacial Properties of Electron Beam Cured Composites*

ID: ORL99-08
PI: Christopher Janke
Engineering Technology Division
Phone: 423 574-9247
Partners:
Acsion Industries, Inc., Pinawa, MB, Canada
Adherent Technologies, Inc., Albuquerque, NM
Applied Poleramic Inc., Benicia, CA
Boeing Phantom Works, Seattle, WA
BP Amoco Chemicals, Alpharetta, GA
E-BEAM Services, Inc., Princeton, NJ
Hexcel, Salt Lake City, UT
Lockheed Martin, Fort Worth, TX
STERIS Isomedix Services, Libertyville, IL
UCB Chemicals Corporation, Smyrna, GA
YLA, Inc., Benicia, CA

FY 99 Funding: $125K
Total Project Funds: $750K

Background

Electron Beam curing of composites and adhesives is a nonthermal, nonautoclave curing process which offers substantially reduced manufacturing costs and curing times, improvements in part quality and performance, reduced environmental and health concerns, and improvements in material handling, as compared to conventional thermal curing. As satisfactory properties of electron beam cured composites are achieved, U.S. industry expects rapid implementation of these materials for making better, less expensive, and lightweight airplanes, spacecraft, and automobiles.

Research Objective

Oak Ridge National Laboratory, NASA's Langley Research Center, and eleven industrial partners have pooled their resources to understand and resolve the fiber-resin interface property deficiencies in electron beam cured composites.

Previous research on electron beam cured composites has shown that interface dependent properties, such as composite interlaminar shear strength, are generally lower than those of high performance, autoclave cured composites. A primary objective of this project is to determine the chemical, physical, and/or mechanical mechanisms responsible for poor adhesion between carbon fibers and epoxy resins subjected to electron beam processing. Another important objective is to optimize electron beam compatible carbon fiber surface treatments, chemical agents, modified radiation curable epoxy resin systems, and improved fabrication and processing methods for producing electron beam cured composites having excellent interfacial properties. Currently, work is focussed on characterization of the carbon fiber-epoxy resin interface and identification of the critical radiation processing parameters that influence the properties of electron beam cured composites. Additionally, various chemical agents, including coupling agents and reactive finishes, which are specifically designed to improve the fiber-resin adhesion properties, are being evaluated. The project complements DOE investments in advanced materials research, and research on energy efficiency and environmental stewardship.

17: *Development of High-Temperature Superconducting Wire Using RABiTS Coated Conductor Technologies*

ID:	ORL 97-02
PI:	David Christen Solid State Division
Phone:	423 574-6269
Partner:	Minnesota Mining and Manufacturing Company St. Paul, MN Southwire Company Carrollton, GA
FY 99 Funding:	$250K
Total Project Funds:	$750K

Background

High-temperature superconducting (HTS) materials have virtually no resistance to electric current. Accordingly, they hold promise for greatly improved energy efficiency in a number of power applications related to the production, distribution, storage, and utilization of electric energy.

Research Objective

This collaboration between Oak Ridge National Laboratory, 3M Company, Southwire Company, and Los Alamos National Laboratory is pursuing the fabrication and scale up of long-length coated conductors that can provide operating characteristics currently unattainable by *any* electrical conductor. The focus of the project is on both the simplification and optimization of oxide buffer layers on reactive metals in general, and specifically development of a simplified ex-situ approach to the co-evaporation and processing of the superconductor coatings.

Results

This project is based on a recent breakthrough at ORNL, referred to as RABiTS (Rolling Assisted Biaxially Textured Substrates). In this process, pure nickel is roll-textured and heat treated to produce a single crystal-like substrate. Next, extremely thin layers of two ceramic materials are deposited epitaxially using a laboratory-scale electron beam system. A cerium oxide layer as thin as 100 angstroms is then deposited on the nickel substrate, followed by a 1400 angstrom layer of yttria-stabilized zirconia. In the laboratory environment, this layer takes about 20 minutes to grow. The HTS material is then deposited, completing the process. The buffer layers produced to date have excellent micro-structural characteristics. 3M is actively developing the scale-up of these techniques for the production of long-length HTS tapes in a "continuous" process. Implementation of these tapes will produce superconducting transmission lines capable of 2-5 times the power transfer into urban areas, without need for additional rights-of-way and without significant losses to resistance. Other applications, such as power transformers, motors, current limiters, and magnetic energy storage are projected to produce markets of tens-of-billions of dollars per year. This project supports DOE's efforts in materials research and energy related technologies.

Award

1. 1999 R&D 100 Award.

Publications

1. Q. He et al, *Physica C*, vol. 275, 155 (1997).
2. M. Paran-thaman et al., *Physica C*, Vol. 275, 1997, 266, (1997).
3. A. Goyal et al., *MICRON*, submitted 1999.
4. R. Feenstra, A. Goyal, D. K. Christen, M. Paranthaman, D. F. Lee, D. Verebelyi, E. D. Specht, J. D. Budai, D. P. Norton, and D. M. Kroeger, *Science*, submitted 1999.

Patents

1. US Patent No. 5,741,377
2. US Patent No. 5,739,086

18: *Atomic Scale Structure of Ultrathin Magnetic Multilayers and Correlation with Resistance, Giant Magnetoresistance, and Spin-Dependent Tunneling*

ID:	ORL97-03	
PI:	Bill Butler Metals and Ceramics Division	
Phone:	423 574-4845	
Partner:	Honeywell Solid State Electronics Center Plymouth, MN	
FY99 Funding:		$250K
Total Project Funds:		$750K

Background

Giant Magnetoresistance (GMR) and Spin-Dependent Tunneling (SDT) are two recently discovered phenomena that are providing important new insights into how spin affects the transport of electrons in materials. Both phenomena also have the potential to spark revolutionary advances in several important technologies. Both require the controlled deposition of ultrathin films. In order to realize the scientific and technological potential of these phenomena, it is necessary to relate the spin-dependent transport properties to the spin-dependent electronic structure of the deposited structures. Recent advances in electronic structure theory allow us to calculate spin dependent transport, at least for ideal thin film structures. The missing key to advancement of this field is lack of atomic scale characterization of the deposited films.

Research Objective

This collaboration between ORNL and Honeywell will determine the physical, chemical, and magnetic structure of GMR and SDT films and relate their structure to their magnetic and transport properties. To achieve this goal, the project combines a uniquely powerful set of characterization tools: X-ray Reflection and Diffraction, Atom-Probe Microscopy, Z-Contrast Electron Microscopy with Electron Energy Loss Spectroscopy, Electron Holography, and Superconducting Quantum Interference Magnetometry, with first principles computer codes, that are capable of calculating the spin dependent conductivity for realistic systems.

Results

The project has provided important insights into the physical, chemical, and magnetic structure of GMR and SDT systems. X-ray analysis has been used to investigate film texture and pointed out the need for better control of the phase of the underlying tantalum seed layer. Measurements and calculations of the effects on magnetic properties of the tantalum capping and seed layers pointed out the advantages of replacing the tantalum capping layer by a different material. Temperature measurements of the magnetic switching behavior indicated a potential problem in the design and operation of the devices. Electron-holography was used to obtain images of the fringing fields near the submicron scale magnetic memory cells. The most important advance has been the development of an exciting new technique that will use atom probe field ion emission microscopy to obtain a three-dimensional atomic scale reconstruction of the structure of the magnetic multilayer films and their interfaces. The project supports DOE investments in advanced materials research.

Award

1. Microscopy Society of America Advances in Instrumentation and Techniques, First Prize 1999.

Publications

1. W. H. Butler, X.-G. Zhang, T. C. Schulthess, D. M. C. Nicholson, A. B. Oparin, and J. M. MacLaren, *Journal of Applied Physics*, 85**,** 5834 (1999).
2. D. J. Larson, A. K. Petford-Long, A. Cerezo, D. T. Foord, T. C. Anthony and M. K. Miller *Microscopy and Microanalysis*, 5, 150 (1999).
3. M. Kowalewski, E.D. Specht, W.H. Butler, N. Moghadam, G.M. Stocks, T.C., Schulthess, K.J. Song, J.R. Thompson, A.S. Arrott, T. Zhu, J. Drewes, R.R. Katti, M.T. McClure, and O. Escorcia, *Journal of Applied Physics*, submitted 1999.
4. S. Arrott, Y. Lu, R. Katti, J. Sather, D. Schipper, T. Zhu, M. Kowalewski, K.J. Song, and J.R. Thompson, W.H. Butler, *Journal of Applied Physics*, submitted 1999.
5. D. J. Larson, R. L. Martens, T. F. Kelly, M. K. Miller, N. Tabat, *Journal of Applied Physics*, submitted 1999.

19: *Evaluation of Fluid Catalytic Cracking Feed Nozzles*

ID:	ANL95-09
PI:	Rajesh Ahluwalia Technology Development Division
Phone:	630 252-5979
Partners:	Phillips Petroleum Company Bartlesville, OK UOP Research Center Des Plaines, IL Amoco Corporation Naperville, IL Chevron Richmond, CA
FY99 Funding:	$40K
Total Project Funds:	$750K

Background

Approximately 50% of the US gasoline pool is processed through fluid catalytic cracking (FCC) units. Although the importance of feed nozzle atomization to the yield of FCC units is widely recognized, quantitative data on nozzle performance are not available. Improved nozzle efficiency will result in dramatic cost reductions for gasoline production.

Research Objective

The goal of this project between Argonne National Laboratory and the industry partners was to address this lack of knowledge by characterizing the performance of commercial feed nozzles using state-of-the-art laser-optics instrumentation. The performance data will allow companies to select commercial nozzles that are optimal for their feeds and operating conditions. The project supports DOE initiatives to apply high performance computing to advanced exploration, production, and processing technologies, which will enable domestic producers to lower finding and development costs.

Results

A total of five FCC nozzles have been tested. The operating maps for these nozzles showed the actual performance in terms of air and water flow rates and pressures required to produce those flows. The spray jets were completely characterized in terms of the spray angle, volume flux, 3-D velocities, and droplet velocity vector. The resulting database defines the fine structure of the spray jets in terms of flow asymmetries, appearance of secondary volume flux peaks, and the growth of the jet boundary. Nozzles were tested for at least one air-water ratio. Most nozzles were characterized at a second air-water ratio for comparison. Particular attention was paid to the changes in spray structure caused by an increase or decrease in assist air. In a complementary task, a state-of-the-art multi-component droplet vaporization model was formulated to determine the impact of atomization parameters on the overall yield of FCC units. It includes heat and mass transfer processes in the droplet and gas-phase boundary layer, equations for droplet size, velocity and position, droplet-gas phase interactions, and droplet-catalyst interactions. A parametric study was conducted to calculate droplet lifetime and penetration distance as a function of droplet size. Initial droplet and gas temperatures and velocities were also modeled. The calculations were performed for oil compositions representative of heavy and light feed stock. The results illustrated the importance of convective heating of droplets, radiative heat transfer from hot catalyst particles, and contact heating due to collision between oil droplets and catalyst particles.

Publications

1. V. J. Novick, R. K. Ahluwalia, K. Dockus, K. W. Flanagan, D. Franklin, R. C. Haglund, K. J. Peterson, ANL Report, July 1997.
2. V. J. Novick, ., R. K. Ahluwalia, K. W. Flanagan, Haglund, R. C., K. J. Peterson, ANL Report, December 1997.
3. V. J. Novick, R. K. Ahluwalia, R. C. Haglund, R. Kumar, J. L. McCuin, D. Potirala, ANL Report, February 1999.
4. V. J. Novick, Y. Wang, R. C. Haglund, R. K. Ahluwalia, ANL Report, May 1999.
5. V. J. Novick, Y. Wang, R. C. Haglund, R. K. Ahluwalia, ANL Report, August 1999.

20: *Synthesis and Crystal Chemistry of Technologically Important Ceramic Membranes*

ID:	ANL97-06	
PI:	James Jorgensen Materials Science Division	
Partner:	Amoco Naperville, IL	
Phone:	630 252-4250	
FY99 Funding:		$195K
Total Project Funds:		$510K

Background

Achieving the conversion of natural gas to synthesis gas (syngas, a mixture of CO and H_2) using oxygen-permeable ceramic membranes would bring vast resources of natural gas, available in the north slopes of Alaska, within economic reach. Since natural gas has lower green house gas emissions than petroleum liquids, increased natural gas use will diversify energy supplies and lower environmental emissions. One potential route to this new technology depends on the development of suitable ceramic membrane materials.

Research Objective

Argonne National Laboratory and Amoco are developing oxygen-permeable ceramic materials and are evaluating materials performance in a prototype reactor to demonstrate the commercial viability of the gas conversion process. The project objective is to develop a cost effective technology for conversion of natural gas to liquid fuels. The project is investigating materials used in membranes in current reactors, and the performance of membranes having novel compositions. Additionally, membrane crystal chemistry and structure changes during gas conversion are being examined. The research combines DOE missions in advanced materials characterization and renewable energy sources.

Results

A ceramic membrane material, based on Sr-Fe-Co-O, has been developed and has demonstrated suitable transport properties and survivability in the reactor environment. However, prior to the initiation of this project, neither the exact chemical composition nor crystal structure of this material were precisely known. The phases present in this material have been identified, and their compositions, crystal structures, and transport properties have been characterized. These studies provide an understanding of which phases are responsible for desirable transport properties and which phases contribute to mechanical and chemical stability. Such fundamental studies are helping to develop new compositions with improved functional properties. In-situ neutron powder diffraction, under conditions that simulate a working reactor environment, is being used to learn how the material changes at high temperature when the oxygen partial pressure is varied over a wide range, and what structural/chemical changes are associated with degradation of the material during operation. This information is being used to optimize the synthesis and processing of the membrane material. Methods have been developed for fabricating ceramic tubes that are suitable for use in a prototype reactor.

Publications

1. B. Ma, U. Balachandran, J. P. Hodges, J. D. Jorgensen, D. J. Miller, J. W. Richardson, *Jr. Mat Lett.*, 35, 303 (1998).
2. 1. B. Ma, U. Balachandran, B. J. Mitchell, J. W. Richardson, J. P. Hodges, J. D. Jorgensen, *Mater. Res. Soc. Sym. Proc.*, Vol. 496, 167-172, Pittsburgh, P. A., 1998.
3. J. P. Hodges, J. D. Jorgensen, D. J. Miller B. Ma, U. Balachandran, J. W. Richardson, *Mater. Res. Soc. Sym. Proc.*, Vol. 496, 173-178, Pittsburgh, P. A., 1998.
4. B. Ma, J. P. Hodges, J. D. Jorgensen, D. J. Miller, J. W. Richardson, U. Balachandran, *Mat. Res. Bull.*, 35, 303 (1998).

21: *Development of Electrolyte and Electrode Materials for Rechargeable Lithium Batteries*

ID:	BNL98-04
PI:	Xiao-Qing Yang Deptartment of Applied Science
Phone:	516 344-3663
Partner:	Gould Electronics, Inc. Eastlake, OH

FY99 Funding:	$250K
Total Project Funds:	$650K

Background

Enhancing performance, reducing cost, and replacing toxic materials by environmentally benign materials are strategic goals of DOE in lithium battery research. Development of new electrolyte materials, aza and boron based anion receptors as additives, organic lithium salts, and plasticizers is aimed at enhancing the conductivity and lithium transference number of lithium battery electrolytes and reducing the use of toxic salts in these electrolytes.

Research Objective

In this project, electrolyte materials and cathode materials, developed at Brookhaven National Laboratory, will be evaluated by Gould for potential use in commercial battery cells. The objective of the project is to develop these electrolyte and cathode materials for rechargeable lithium batteries, especially for lithium ion and lithium polymer batteries. The research targets optimization of boron-compound-based composite electrolytes, and synthesis of new lithium salts and plasticizers for polymer and polymer gel electrolytes.

Results

Characterization of cathode materials will be carried out utilizing the National Synchrotron Light Source. In-situ x-ray absorption and x-ray diffraction techniques, developed at BNL, will be used to probe the relationship between performance and the electronic and structural characteristics of intercalation compounds such as $LiNiO_2$, $LiCoO_2$, and $LiMn_2O_4$ spinel.

The Gould team has produced and chosen some promising materials and has defined the overall performance requirements. New cathode materials, such as $LiNi_{0.8}Co_{0.2}O_2$, $LiNi_{0.8}Co_{0.2-z}Al_zO_2$, and $LiNi_{0.7}Mg_{0.125}Ti_{0.125}O_2$, have also been studied. These results will be used to guide new material selection and quality control procedures for Gould. Successful research will result in the development of less expensive and more environmental friendly lithium battery materials for commercial applications. The project marshals DOE's investment in basic materials research to promote economically and environmentally desirable new processes and materials for energy use.

Publications

1. S. Mukerjee, T. R. Thurston, M. Jisrawi, X. Q. Yang, J. McBreen, M. L. Daroux,and X. K. Xing, *Journal of the Electrochemical Society*, 145, 466 (1998).
2. X. Q. Yang, X. Sun, S. J. Lee, S. Mukerjee, J. McBreen, M. L. Daroux ,and X. K.Xing, *Electrochemical and Solid State Letters*, 2, 157 (1999).
3. H. S. Lee, X. Q. Yang, C. Xiang, J. McBreen, L. S. Choi, *Journal of the Electrochemical Society*, 145, 2813 (1998).
4. X. Sun, H. S. Lee, S. Lee, X. Q. Yang,, and J. McBreen, *Electrochemical and Solid State Letters*, 1, 239 (1998).
5. J. McBreen, S. Mukerjee and X. Q. Yang, *Synchrotron Radiation News*, 11, 18 (1998).
6. Y. Ein-Eli, S. H. Lu, M. A. Rzeznik, S. Mukerjee, X. Q. Yang, and J. McBreen, *Journal of the Electrochemical Society*, 145, 3383 (1998).
7. H. S. Lee, X. Q. Yang, C. Xiang, J. McBreen, J. H. Callahan and L. S. Choi, *Journal of the Electrochemical Society*, 146, 941 (1999).
8. Y. Ein-Eli, J. T. Vaughey, M. M. Thackeray, S. Mukerjee, X. Q. Yang, and J. McBreen, *Journal of the Electrochemical Society*, 146, 908 (1998)
9. X. Q. Yang, X. Sun, and J. McBreen, *New Findings Electrochemistry Communications*, 1, 227 (1999).
10. M. Giorgetti, S. Passerini, W. H. Smyrl, S. Mukerjee, X. Q. Yang, and J. McBreen, *Journal of the Electrochemical Society*, 146, 2387 (1999).

22: *Development and Validation of a Computational Fluid Dynamic (CFD) Simulation of a Novel Fluid Catalytic Cracker (FCC) Process*

ID:	ANL99-07
PI:	Shen-Lin Chang Energy Systems Division
Phone:	630 252-6955
Partner:	Process Innovators, Inc. Salt Lake City, UT
FY 99 Funding:	$125K
Total Project Funds:	$750K

Background

The Low-Profile Fluid Catalytic Cracking (LPFCC) pilot plant is an improvement in fluid catalytic cracking technology that converts heavy fractions of crude oil to more useful products. The low-profile technology uses a smaller plant design that lowers construction and operating costs and allows refiners to control a number of variables that are not controllable in conventional FCC units. This enables smaller oil refineries to maximize product yield, cut production costs, and be more competitive with larger refineries. Computer simulation is one method of developing an understanding of the impact of design and operating parameters on the pilot unit's performance.

Research Objective

Argonne National Laboratory and Process Innovators, Inc are developing a computational fluid dynamics (CFD)-based computer simulation of a novel Low Profile Fluid Catalytic Cracking (LPFCC) process technology. The software will (1) evaluate/interpret data derived from a small pilot-scale (1000-bbl/day) unit being installed in the Flying J. Inc., refinery and (2) conduct parametric, sensitivity, and optimization studies in support of further scale-up/commercialization activities.

ANL will modify its multiphase, reacting-flow ICRKFLO code to simulate a multistage FCC system. The 1000-bbl/day pilot-scale unit will be instrumented, and requisite product analysis will be undertaken to provide the database needed to validate the simulation. The 1000-bbl/day unit will be operated over a broad range of temperatures, catalyst/oil mass ratios, catalyst activity, and residence times in both upflow and downflow modes. The project also has a major scientific objective, namely, to advance the "state of the art" in multiphase, reacting flow computational fluid dynamics. Validating the staged, low-profile L/D riser simulation by means of experimental data represents a major scientific accomplishment, because the focus is on complex coupled hydrodynamic/kinetic phenomena that occur in the critically important mixing zone. The database that will evolve from the one-year test program will be unique in that both upflow and downflow tests will be run on the same system, over identical parametric ranges. Also, critical phenomenological models that have been developed and incorporated into the ICRKFLO code will be validated under new and challenging operating conditions. Successful validation of the multiphase reacting flow simulation of the riser would underscore the applicability of ANL's code to a variety of processes in the petroleum and chemical industries. The project supports the DOE's initiative to increase demand for US produced petroleum resources through research using high performance computing.

23: *Automotive Underhood Thermal Management Analysis Using 3-D Coupled Thermal-Hydrodynamic Computer Models*

ID:	ANL98-14
PI:	David Weber Reactor Engineering Division
Phone:	630 252-4576
Partners:	Analysis and Design Applications Company (ADAPCO) Melville, NY Supercomputer Automotive Applications Partnership (SCAAP) c/o Ford Motor Company Dearborn, MI
FY99 Funding:	$200K
Total Project Funds:	$750K

Background

The underhood of most contemporary vehicles presents an adverse environment for the operation of sensitive components. As more and more components are added to the engine, the need to understand and manage the thermal loads under the hood become critical. Vehicle manufacturers have recognized that it is desirable to replace the current practice of building and testing expensive prototypes with a numerical approach that can quickly and effectively analyze various designs and direct the designers toward the most efficient solutions.

Research Objective

The purpose of this project, conducted by Argonne and its industry partners, is to develop an Underhood Thermal-Hydrodynamic Integrated Model which will be based on the CHAD code. This code was developed specifically for the analysis of hydrodynamic phenomena in complex geometries, and was selected as the analysis tool by the USCAR Supercomputer Automotive Applications Partnership (SCAAP).

The focus of this project is to develop and integrate thermal models for convective, conductive, and radiative heat transport, and models for critical heat management system components. The project supports the DOE's initiative to develop more energy efficient vehicles. DOE high performance computing and mathematical sciences programs will also benefit from modeling, simulation advances, and form development of numerical algorithms for execution on parallel computers.

Results

A fan model to predict velocity distribution past fan blades has been developed. This model is being implemented into the CHAD code, and validated against experimental data. A preliminary version has been provided to ADAPCO for evaluation and implementation into their commercial computational fluid dynamics (CFD) code, STAR-CD. The radiator model being developed will treat the air side, the wall side and coupling through thermal structures. Initial calculations have been performed with STAR-CD to develop an appropriate implementation strategy for CHAD. A third ANL focus area is performance optimization of the CHAD CFD code. CHAD has now been compiled with the portable extensible tool kit for scientific computation (PETSc) software suite. PETSc logging functions have been used to monitor performance and special solvers have been used in the pressure iteration. Detailed performance results were presented, leading to the conclusion that improved data clustering and utilization of advanced Newton-Krylov solvers are likely to improve performance substantially.

24: *Controlled Non-Isothermal Hot Forging Using Infrared for Microstructural Control and Energy Savings*

ID:	ORL98-08
PI:	Craig Blue Metals and Ceramics Division
Phone:	423 574-4351
Partner:	A. Finkl and Sons Chicago, IL Forging Industry Association Cleveland, OH Scientific Forming Technologies Corporation Columbus, OH
FY99 Funding:	$225K
Total Project Funds:	$495K

Background

Hot forging is a dominant commercial method for the production of net- and near net-shape components from a large number of metals and alloys which are ultimately used in many consumer products such as automobiles and hand tools. Forging is a $50 billion industry in the United States and employs 400,000 people. Infrared heating is of great interest to the steel, metal casting, heat treating, and particularly the forging industry because it offers the opportunity to decrease costs and improve the properties of parts. Infrared heating allows control of thermal gradients in a forging billet, permits optimal control of forging deformation, and minimizes total heating requirements.

Research Objective

The objective of this project between ORNL and the industry partners is to develop a fundamental understanding of infrared heating as applied to the forging industry. This will permit improved control of forged part structure and properties and lead to reduced production costs. Two areas of particular interest to the forging industry are nonisothermal forging (heating for restrikes) and extended die life. These interests will be explored through: (1) the development of experimental absorption data for input into thermal modeling of a given geometry/part prior to forging; (2) applying deformation modeling in conjunction with thermal modeling to optimize the forging cycle (including restrikes) with respect to microstructure and energy consumption; (3) verification of thermal and deformation modeling with existing infrared and forging equipment; and (4) incorporation of microstructural analysis with an existing deformation modeling package. Infrared heating will allow economical forging of restrikes for the first time in the forging industry while delivering optimized part microstructures and large energy savings. The project goals support the DOE's initiatives to develop energy efficient industrial processes.

Results

The experimentation on infrared preheating of forging was initiated and finished during 1999. Thermal modeling was utilized in order to predict the type of heating rates to be obtained by the 20-40 watts/cm^2 which can be produced by an infrared flat bank array. This was also accomplished in order to ensure that preferential surface overheating and annealing would not occur. The Forging Industry Association supplied a fully instrumented die for the infrared preheating work. The results of this study revealed that infrared preheating can be performed reproducibly with uniformity and shorter heating time than by using conventional methods. Experimental and predicted results matched extremely well and confirmed that the limiting step in die preheating is thermal conduction through the die thickness. Based on these results, the industrial partners requested and received technical guidance for the development of an inexpensive in-die preheating system. Also, in-house testing of infrared preheating and post annealing of reworked Komtek dies, over a 1.5 weeks period, have been accomplished. Thermal modeling of cylindrical aluminum billets and flat steel specimens were accomplished in order to reveal possible attainable gradients utilizing infrared heating. Infrared heating experiments were performed on these materials to confirm modeling and generate needed infrared absorption data.

25: *Advanced Computational Models and Experiments for Deformation of Aluminum Alloys - Prospects for Design*

ID:	PNL99-07
PI:	M.A. Khaleel
Phone:	509 375-2438
	Virtual Prototyping and Engineering Simulations Laboratory
Partners:	Alcoa, Inc.
	Alcoa Center, PA
	Analysis Research Inc.
	Palo Alto, CA
	National Institute of Standards and Technology
	Gaithersburg, MD
FY99 Funding:	$125K
Total Project Funds:	$750K

Background

Why and how do metals deform, bend, twist, and break? The answer lies in our ability to understand basic mechanisms and phenomena that operate at a very small length scale, micro meters, or even nanometers. Dislocations are the basic lattice line defects in crystalline materials, with defect densities as high as $10^{15}/m^2$. This project aims at understanding their collective and complex nonlinear dynamical behavior by merging a set of highly sophisticated experiments, using computer aided, massive numerical analyses, and experimental data. The project impacts future computational and experimental advances in dislocation theory and elevates prospects for predictive alloy properties control. Application of this research to manufacture and design of existing and new lightweight Al materials supports DOE's initiatives in high performance computing.

Research Objective

Pacific Northwest National Laboratory in collaboration with the industry partners will develop a framework for predicting the characteristics of plastic deformation of single crystals. This model will provide a means of predictive control of the alloy microstructure to yield specific ranges of engineering properties. The project has two main tasks. The first task is to develop and integrate plastic deformation models at discrete defect and single crystal scales. This includes advancing a three-dimensional dislocation dynamics model, developing a strain percolation model, and conducting a comprehensive set of experiments to verify specific aspects of and provide input to all modeling scales. The second task is to use an overall framework to predict the full stress-strain response of a pure Al and two binary alloy single crystals, and to develop a methodology for selection and control of the alloy properties. The project is currently evaluating a series of Aluminum solid solution alloys as a screening test to determine which alloy systems should be used for dislocation studies. The team has been developing a mechanical testing apparatus and protocols for shear testing of single crystals, in-situ transmission electron microscope deformation of pre-deformed samples, and evaluation of deformation structures.

26: *Mathematical Simulation of Glass Production*

ID:	PNL98-10	
PI:	George Fann Environmental Health and Sciences Division	
Phone:	509 375-6446	
Partner:	Corning, Inc. Corning, NY IBM Waltham, MA	
FY 99 Funding:		$250K
Total Project Funds:		$625K

Background

Simulation of glass production requires solving partial differential equations which incorporate advection and strong dissipation of energy. Additional difficulties are that a number of boundary conditions at interfaces have to be imposed, and appropriate conditions have to be found for specific applications. However, accurate models and robust computational techniques, as well as a scalable parallel implementation on massively parallel computers, will assist DOE"s design and production efforts in vitrifying high level radioactive waste, as well as projects involving manufacturing of materials. For US industry, the success of such models will assist production engineers in designing and reducing the cost of producing higher quality glass and optical products. This cross-section of beneficiaries is a result of DOE initiatives to increase the competitiveness of US industry through use of high performance computing.

Research Objective

The goal of this collaborative project between Pacific Northwest National Laboratory, Corning, and IBM is to produce mathematical models and software for parallel computers to simulate the production of glass products that are beyond the capability of existing commercial software.

Analytical and numerical models and methods for multi-phase flow with free and moving boundary conditions are being explored and developed for liquid glass. Validation and assessment of numerical models and analytical results are being performed using experimental data. Two scales of fluid models are being investigated and will be asymptotically matched. Software based on representation of differential operators in multi-wavelet bases will be developed as a basis for an adaptive solver for fluid equations. A new mesoscale dissipative particle dynamics solver will be developed to model the microstructure and composition of complex fluids that are beyond the macroscopic boundary conditions commonly used in fluid simulations.

Results

In its first year, the project has demonstrated that multi-wavelet bases are well suited for high-order adaptive solvers of certain classes of partial differential equations and may present a better choice than other wavelet bases. The representation of differential operators in these bases may be viewed as multi-resolution generalization of finite difference schemes, discontinuous finite element schemes, and finite spectral elements. The mesoscale dissipative particle dynamics solver is being developed and has been applied to the study of thin films. Upscaling of mesoscale simulation to the continuum model is being investigated using kinetic theory formulae.

Publications

1. Dzwinel, W., Alda, W., Pagoda, M. Yuen, D.A., *Physica D*, accepted 1999.
2. Dzwinel, W., Yuen, D.A., *Molecular Simulation*, 1999.
3. Dzwinel, W., Alda, W., Yuen, D.A., *Molecular Simulation*, accepted 1999.
4. Dzwinel, W., Kitowski, J., Moscinski, J., Yuen, D.A., *IEEE Transaction on Evolutionary Computing*, submitted 1999.

27: *Development of a High Current, High Gradient, Laser Excited, Pulsed Power Electron Gun*

ID:	BNL99-12
PI:	Triveni Srinivasan-Rao Instrumentation Division
Phone:	516 344-5072
Partner:	Brookhaven Technology Group Stony Brook, NY
FY 99 Funding:	$125 K
Total Project Funds:	$750 K

Background

High brightness electron beams are needed for high luminosity electron colliders and efficient, short wavelength Free Electron Lasers. Current technology uses laser excited RF injectors with accelerating gradients up to 100 MeV/m. Electron beams with 100 A current and ~ 2 mm-mrad emittance are routinely achieved with these devices. However, in order to increase the brightness further, new techniques are needed to overcome limitations imposed by variation of the electric field in the RF injectors.

Research Objective

Brookhaven National laboratory and the Brookhaven Technology Group will develop a compact, low cost, high brightness electron gun. The project will overcome limitations in the current technology by use of a new injector design combined with a very high accelerating field, kept constant over the spatial and temporal extent of the electron beam. A high voltage pulse will be applied between the electrodes of a suitably designed diode. Photoelectrons liberated from the cathode by irradiation with a short laser pulse will be accelerated to relativistic velocities within one mm from the cathode.

This design, in combination with an accelerating field of 1GV/m, will dramatically reduce density gradients in the electron current. Secondary objectives of the project are electron beam characterization and optimization of the Bremsstrahlung radiation from a high Z material interacting with the electron beam. The high brightness electron beam will be used in linear colliders, short wavelength Free Electron Lasers, and as a test beam for advanced accelerator concepts, as well as a stand-alone device for a variety of biological and medical applications. This device will also act as a test stand for studying the properties of materials in ultrahigh electric fields. The Bremsstrahlung radiation will be useful for imaging hydrated biological specimens, microlithography, and micromachining. The project will advance the DOE's high energy and nuclear physics programs in subatomic particle physics.

28: *Development of Multi-Channel ASICs for CdZnTe Gamma Detector Arrays*

ID:	BNL 97-06	
PI:	Paul O'Connor Instrumentation Division	
Phone:	516 344-7577	
Partner:	eV Products Saxonburg, PA	
FY99 Funding:		$122K
Total Project Funds:		$652K

Background

Cadmium Zinc Telluride (CZT) array detectors are the only solid-state detectors available for X and gamma rays in the 20 - 150 keV energy range, and as such play an important role in systems where size and weight are important requirements. There is a large need for solid state gamma and X-ray imaging capability for both medical and industrial applications. Solid state CZT arrays with application-specific integrated circuit (ASIC) readouts can form the basis of a portable nuclear medicine camera, a handheld interoperative probe for cancer surgery, bone densitometry scanners for the detection of osteoporosis, explosives detectors for security screening, and high speed defect imagers for manufacturing lines.

Research Objective

Brookhaven National Laboratory and eV Products are applying new microelectronics technology to enhance the attractiveness of CZT arrays to the field of industrial/medical imaging. To this end, the goal of the project is to miniaturize the front-end electronics. CZT detectors are produced with hybrid circuit readout electronics, which occupy an area of about 2 square inches for each channel. By implementing the electronics functions as an ASIC, a 16-channel readout on a single chip measuring 5 mm on a side will be produced.

Low-noise ASIC circuit elements will benefit DOE's high energy and nuclear physics programs. Additionally, the technology will enhance the DOE's medical sciences initiatives for the development of non-invasive, biological imaging technologies.

Results

BNL has adapted low-noise designs to ASIC technology, with applications to detectors for the relativistic heavy ion collider and the large hadron collider. This project will develop several custom chips which will be tailored to the industry partner's product needs. During FY97 and FY98, BNL designed and produced 5 low noise preamplifier/shaper ASICs. These chips are intended to achieve excellent resolution by means of low noise front end design, detector leakage current compensation, baseline restoration, and high power supply rejection. Several new circuit blocks have been invented and successfully applied to solve these problems. The fabricated ASICs have been coupled to CZT detectors, and their performance meets the needs of eV Products' applications.

Publications and Presentations

1. G. De Geronimo, P. O'Connor, Charge preamplifiers in scaled CMOS. Invited for Presentation at Nuclear Science Presentation at Nuclear Science Symposium, Seattle, 1999.
2. P. O'Connor, G. De Geronimo, A CMOS detector leakage current self-adaptable continuous reset system. Presentation at Nuclear Science Symposium, Seattle, Oct. 99.
3. G. De Geronimo, P. O'Connor, *Nuclear Instruments & Methods*, A421, 322 (1999).

29: *Microcircuits and Sensors for Portable, Low-Power Data Collection and Transmission*

ID:	BNL 97-07	
PI:	Paul O'Connor Instrumentation Division	
Phone:	516 344-7577	
Partner:	Symbol Technologies, Inc. Holtsville, NY	
FY99 Funding:		$0
Total Project Funds:		$750K

Background

Small, inexpensive radio transceivers will have applications in the following: large detectors used in high energy physics colliders, where many thousands of subdetector elements need to communicate; wireless networks which will allow data collection from remote or hazardous areas; and providing a means for mobile access to large databases.

Research Objective

Brookhaven National Laboratory and Symbol Technologies are producing an inexpensive single-chip frequency agile RF transceiver operating in the 2.4 GHz range - a universally accepted unlicensed band - with data rates up to 250 kbps and an approximate range of 50 feet. This "radio on a chip" will play an important role in cost reduction in Symbol's existing wireless data terminal product line and offers the possibility of lightweight, cordless bar code scanners. The goal of this project is to achieve acceptable radio frequency performance from standard industrial complementary metal oxide semiconductor (CMOS) technology. The BNL-Symbol team has successfully fabricated a fully integrated transmitter based on a phase-locked loop frequency synthesizer. With this chip, a live wireless link was demonstrated between a scanner and an existing Symbol wireless data terminal, operating over a distance of up to 60 feet. Error-free transmission was obtained at a data rate of 19.6 kbps.

Results

During FY99, research was concentrated on key receiver circuit blocks. A first prototype of a direct-conversion receiver was designed, fabricated, and tested, incorporating a synthesized local oscillator, downconversion mixers, and baseband circuitry. A parallel effort led to the first demonstration of a low noise amplifier (LNA) with an integrated mixer. The work plan for the current year includes the optimization of the LNA and mixer blocks, a new digital fractional-N frequency synthesizer, and migration of all the circuits to the most recent 0.35 micron CMOS technology. The technology being developed in this project, if successful, will enable the production of wireless data links at very low cost. Thus, commercial applications exist in all areas of information technology, especially portable, battery operated communications and computing devices. For Symbol, these chips will allow cost reduction of their existing wireless local area network products and introduction of wireless capability on their small, portable scanners. The project will benefit DOE's high energy and nuclear physics programs through development of high performance instrumentation.

Presentations

1. G. De Geronimo, P. O'Connor, "A novel CMOS Class AB Rail-to-Rail Output Stage". Nuclear Science Symposium, Seattle, Oct. 99.
2. G. De Geronimo, P. O'Connor, J. Grosholz "A Novel CMOS Baseline Holder for Readout ASICs". Nuclear Science Symposium, Seattle, Oct. 99.
3. G. De Geronimo, P. O'Connor, "A generation of Novel Readout ASICs for CZT Detectors". Nuclear Science Symposium, Seattle, Oct. 99.

30: *High Performance System Area Networking*

ID:	LBL99-20	
PI:	Bill Saphir	
Phone:	510 486-5442	
Partner:	Intel Corporation Beaverton, OR	
FY99 Funds:		$125K
Total Project Funds:		$750K

Background

VIA is a software and hardware standard that enables low-overhead communication on "system-area" networks (SANs). It is the first such interface with broad industry support, and promises performance improvement over Internal Protocol (IP) by a factor of ten. Moreover, VIA provides functionality not available in IP, such as remote memory operations, that can be significantly accelerated by inexpensive hardware, and can reduce processor overhead by facilitating the overlap of computation and communication. VIA is a critical enabling technology for the next generation of high performance commodity off-the-shelf (COTS) clusters. Such clusters are of interest and importance to the national laboratories for their applications to scientific computing, both numerical and data-intensive. Indeed, they are a leading candidate for the next wave of large-scale scientific computing platforms. High performance clusters are of interest to industry as high-performance servers, presenting an attractive alternative to expensive symmetric multi-processor (SMP) servers with costly and proprietary interconnects, and promising superior fault-recovery and scalability.

Research

This collaboration between Lawrence Berkeley National Laboratory, Argonne National Laboratory, and Intel aims to develop applications, extensions, and implementations of the recently developed Virtual Interface Architecture (VIA) standard. LBNL has developed a high-performance modular implementation of VIA, called M-VIA. To LBNL's knowledge it is the only robust, portable and non-proprietary implementation of VIA, and is the only implementation for Linux, the operating system most commonly used in clusters for scientific computing. Where there is hardware support for VIA, M-VIA provides both the necessary interfaces at the user level and connection management functionality inside the operating system kernel. Where there is no hardware support, M-VIA provides a complete high-performance implementation of VIA. The M-VIA prototype will serve as the basis for a collaborative program to strengthen the viability of VIA, ensure its usefulness for DOE high performance computing applications, and develop cluster computing infrastructure that takes advantage of the high performance offered by VIA. The project will use core technology and expertise from all three collaborators to build infrastructure that is of great importance both to the DOE and to industry. Support of long-term computational and networking research is an important goal of the DOE's advanced scientific computing initiatives.

31: *A High Resolution Subsurface Electromagnetic Imaging Tool*

ID:	LBL94-14	
PI:	Ki Ha Lee	
	Earth Sciences Division	
Phone:	510 486-7468	
Partner:	Baker Atlas	
	Houston, TX	
FY99 Funding:		$152K
Total Project Funds:		$545K

Background

High-resolution subsurface electromagnetic (EM) imaging is critically important for improving the management of petroleum reservoirs and increasing the yield in oil production. The basis of the technology is a new tomographic imaging technique based on a wavefield transform developed at Lawrence Berkeley National Laboratory (LBNL).

Research Objective

The goal of the collaborative effort between LBNL and Atlas Baker is to develop and test a new survey method and instrumentation for high-resolution subsurface electromagnetic imaging. The theoretical basis of the wavefield transform has been known for some time, but has now been generalized to include EM fields, and demonstrated the usefulness of such a transform using a forward model study. In that study, wavefields are first obtained by numerical modeling, and corresponding EM fields are calculated by simple integration of these wavefields. Research at LBNL has focused on solving the inverse problem, in which an observed diffusive EM field is transformed to a wavefield. The velocity of the wavefield is inversely proportional to the square root of the electrical conductivity so that velocity mapping directly leads to conductivity imaging. Once fully developed, the technique should produce electrical conductivity images with a spatial resolution equivalent to that of seismic imaging of the elastic parameter distribution. This technology will enable Baker Atlas to enhance current state-of-the-art knowledge in underground imaging, which should result in increased production by the U.S. oil industry. The new technology will directly help to reduce U.S. energy dependence on foreign oil, complementing core missions of the DOE's Office of Fossil Energy and the Advanced Computational Technology Initiative.

Results

The wavefield transform concept has been verified in a laboratory model study. Wavefield transform software was prepared and delivered to Baker Atlas. A prototype fast pulse transmitter was upgraded to include battery power and optic fiber communication with a detector at the surface. A field test of the prototype transmitter showed that with the use of state-of-the-art electronics and a sophisticated means of noise suppression, it will be feasible to generate field data to which a wavefield transform can be applied.

Publication

1. LBNL Report #43762: Alex Becker, Ki Ha Lee and Lou Reginato, 1999.

32: *Microfabricated Instrumentation for Chemical Sensing in Industrial Process Control*

ID:	ORL97-08
PI:	J. Michael Ramsey Chemical and Analytical Sciences Division
Phone:	423 574-5662
Partner:	Waters Corporation Milford, MA
FY 99 Funding:	$250K
Total Project Funds:	$750K

Background

Researchers at Oak Ridge National Laboratory have shown that microscopic devices can be used to carry out chemical reactions. The work suggests that an entire chemistry laboratory, including chemical containers, beakers for mixing chemicals, and analysis instruments, could be placed on a microchip. Such a microchip laboratory could provide faster, cheaper, and more reliable chemical analyses for environmental monitoring, industrial process control, and medical diagnosis. The devices envisioned could be used as hand portable chemical analysis instruments where samples are analyzed in the field or as emplaced sensors for continuous "real-time" monitoring.

Research Objective

This collaboration between ORNL and Waters Corporation focuses on building microinstruments that can be used for continuous "real-time" monitoring of liquid borne chemical species in industrial process control settings. Specifically, the objective of the project is to develop a microchip device that accomplishes the task of monitoring critical species in water. The device will monolithically integrate filtration structures to eliminate clogging for sample complexity reduction and concentration enhancement, and chemical separations capability for species identification.

Results

Chemical separations on microfabricated structures have been demonstrated with performance that exceeds that provided by conventional laboratory instrumentation. These separations are typically two orders of magnitude faster than conventional separations technology while retaining or exceeding resolving power performance. Solid phase extraction in microfabricated structures has allowed concentration enhancement approaching two orders of magnitude. Additionally, the project has fabricated filtration functional elements for the exclusion of particulate matter. This inlet structure has been used to demonstrate the ability to autonomously sample aqueous materials external to the microchip devices using electrokinetic transport means. Solid phase extraction materials have also been synthesized and tested, using conventional stationary phase supports, for enhanced and selective extraction properties. Tasks which remain include: testing of filtration elements for efficacy in elimination of particles and sampling efficiency, increased solid phase extraction efficiencies, and device integration of the independent functional elements. The resultant technology will have broad application to industrial environmental monitoring problems, such as monitoring municipal water supplies, waste water effluent from industrial facilities, and monitoring of run-off from agricultural activities. This project supports DOE environmental remediation activities and DOE initiatives to develop advanced process technologies for US industry.

Award

1. 1999 Humboldt Award

33: *Dynamic Asynchronous Replication of Object Database Components*

ID:	SLAC99-168	
PI:	Richard Mount Research Division	
Phone:	650 926-2467	
Partner:	Objectivity, Inc. Mountain View, CA	
FY 99 Funding:		$85K
Total Project Funds:		$750K

Background

The Stanford Linear Accelerator Center (SLAC) has been generating larger and larger amounts of high energy physics experimental data. In order that these data be made available to a global network of collaborators, a data base architecture which supports large numbers of users and provides high performance access to large volumes of physically distributed data is critical

Research Objective

Distributed object database technology from Objectivity, Inc. has been chosen by SLAC and the BaBar experiment to support the storage, retrieval, and distribution of hundreds of terabytes of data. To ensure efficient access to the more frequently needed components of the data, it is necessary to replicate these components (objects) and to maintain automatically the consistency of the replicas. The existing Objectivity/DB software from Objectivity, Inc. includes limited support for synchronous automatic data replication; but this feature has been designed with a number of constraints that make it unsuitable for load balancing (auto-determination of the quickest access to data, among distributed databases) or for use in networks with highly variable performance characteristics.

This project will design and implement a new architecture for data replication and load balancing. The first implementations will be tested in the demanding environment of data analysis for the BaBar experiment, after which a robust and widely applicable package will be produced. In addition to its value to the project, a successful implementation will bring vital benefits for the US participation in the Large Hadron Collider high energy physics program at CERN in Geneva. Reliable remote replication of data will ensure that US physicists have full access to the data acquired or processed in Geneva. Objectivity, Inc. anticipates a large commercial market for the asynchronous data replication features. For example, support for distributed access to data with automatic replication and load balancing is critical for the future of global Web-based information systems. Advancing communication capabilities to scientific researchers, funded by the Office of Science, supports DOE's efforts in the mathematical, information, and computational sciences and also serves DOE's large scale networking activities.

34: *Aquatic Plants for Phytoremediation of Toxic Metals and Radionuclides in Sediment*

ID: BNL99-08
PI: Mark Fuhrmann
Deptartment of Advanced Technology
Phone: 516 344-2224
Partner: PhytoWorks
Gladwyn, PA
FY 99 Funding: $125K
Total Project Funds: $750K

Background

Contamination of freshwater marsh environments by metals and/or radionuclides is a frequent problem in the DOE complex and at many other industrial sites. Phytoremediation, the use of plants to decontaminate soil and water, offers a possible solution for future remediation efforts. However, little work has been conducted on the use of aquatic plants for phytoremediation, and a fundamental understanding of the mechanisms and kinetics of contaminant uptake is needed. Remediation and restoration of DOE sites, such as Oak Ridge, and Savannah River, are primary goals of the DOE's and environmental programs.

Research Objective

The purpose of the project is to identify higher plants (rooted epiphytes) that can be used in freshwater, aquatic, and edge environments to remediate sediment that is contaminated with Hg, Ag, and Cs-137 and other contaminants. The objective is to determine mechanisms by which contaminants are taken-up by the plants and then to develop a practical approach to enhancing contaminant concentrations in the plants.

Critical tasks for this project include: (1) identifying aquatic/edge plants that concentrate target contaminants; (2) conducting laboratory microcosm studies using contaminated sediment and both field plants and transgenic plants to identify amendments for increasing bioavailability of pollutants; (3) determining mechanisms of plant uptake of the target contaminants; and (4) genetically engineering selected aquatic and edge plants for enhanced uptake of contaminants. State-of-the-art techniques (e.g. bioengineering) and tools (e.g. synchrotron X-ray microprobe, XANES, and EXAFS) will be used to enhance understanding of how plants interact with the environment. Ultimately, the information generated will allow the identification of plants and uptake mechanisms to be used in a new generation of transgenic plants for phytoremediation. Benefits include the ability to remediate aquatic environments without substantial alteration of the ecosystems.

35: *A Wireless Luminescence Integrated Sensor*

ID:	ORL98-09
PI:	Michael Simpson Instrumentation and Controls Division
Phone:	423 574-8588
Partner:	The Perkin-Elmer Corporation Wilton, CT
FY99 Funding:	$250K
Total Project Funds:	$750K

Backgound

State of the art miniature photo-spectrometers require expensive micromachining techniques. Mass production of these devices requires a large investment in new manufacturing infrastructure, and such devices cost several hundred dollars each. A novel approach, construction of a photo-spectrometer-on-a-chip, is compatible with the existing commercial integrated circuit (IC) infrastructure, and would cost less than $1 each to mass produce.

Research Objective

Oak Ridge National Laboratory and Perkin Elmer are developing a family of wireless, single-chip, luminescence-sensing devices that will impact a number of difficult measurement problems. These wireless luminescence integrated sensors (WLIS) will consist of a microluminometer, a wireless data transmitter, and an RF power input circuit all realized in a standard integrated circuit (IC) process, and a genetically engineered, whole-cell, bioluminescent bioreporter. The encapsulated bioreporter will be deposited directly on the IC to produce a compact, low-power, rugged, low-cost sensor. A rugged, thin-film, bioresistant, biocompatible silicon nitride coating for the IC is also under development. This sensor technology supports DOE programs which develop enabling technologies in environmental monitoring, emergency medical care, and industrial process vessels.

Results

The function of the IC is to detect, filter, amplify, digitize, and report the bioluminescent signal. In effect, the IC serves as a complete laboratory instrument-on-a-chip, called a microluminometer. SiN films with bandgaps above 4 eV (i.e. no absorption of the 490-nm bioluminescent photons), using the molecular-jet chemical vapor deposition (MJ-CVD) process developed at ORNL, have been grown. These films, which are currently undergoing biocompatibility tests, may serve as the protective coating for the IC. The encapsulation work has concentrated on sol-gel as the primary medium. Sol-gel is a silica-based glass that polymerizes under room temperature conditions. Although sol-gel has previously been used to encapsulate yeast cells, the reaction conditions necessary for polymerization (primarily low pH) have previously proven too harsh for bacterial cell immobilizations. Utilizing sonication methods, polymerization under pH conditions conducive to cell survival has been achieved. Both a toluene bioreporter and a naphthalene bioreporter have successfully been encapsulated in sol-gel and shown to produce a fairly significant bioluminescent response. A yeast-based xenoestrogen reporter is also being developed.

Award

1. 1998 Kermit Fischer Environmental Award.

Publications

1. Simpson, M. L., G. S. Sayler, Ripp, S., Nivens D. E.,.Applegate, B. M., Paulus, M. J., Jellison, G. E. Jr., *Trends in Biotechnology*, Vol. 16, 332 (1998).
2. Sayler G. S., Simpson M. L., Nivens, D. E., Ripp, S, Applegate B. M., Paulus M. J., Jellison G. E., *Abstracts of Papers of The American Chemical Society*, submitted, 1999.

Patent Applications

1. "Bioluminescent Bioreporter Integrated Circuit", Simpson, M. L., Sayler, G. S., Paulus, M. J.
2. "An implantable glucose sensor using a bioluminescent bioreporter integrated circuit (BBIC)", Sayler, G.S., Simpson, M. L., Applegate, B. L., Ripp, S.

36: *Microorganism Detection and Characterization*

ID: PNL98-03
PI: Darrell Chandler
Environmental Microbiology Group
Phone: 509 376-8644
Partner: Genometrix, Inc.
The Woodlands, TX
FY99 Funding: $250K
Total Project Funds: $750K

Background

Rapid and accurate detection of pathogenic or disease-causing microorganisms is important in a number of health-related and environmental applications and complements DOE missions in biological research, environmental monitoring, and response to biological weapons.

Research Objective

The objective of this project is to develop a versatile, fully integrated, automated, point-of-use, gene-based detector for broad application in environmental and health related fields. This project is utilizing expertise at Pacific Northwest National Laboratory in nucleic acid extraction and characterization from environmental samples, along with micromachining technology and microfluidic systems. Genometrix is supplying proprietary, patented nucleic acid concentration technology, surface chemistries, and detection arrays.

Results

Genometrix affinity microbead reagents were synthesized and evaluated against "total DNA" binding resins for nucleic acid recovery and PCR amplification (nucleic acid replication) efficacy from four environmental samples, including a concentrated aerosol, surface soil, subsurface sediment, and wastewater sludge. In these samples, humic acids and other compounds that inhibited the Polymerase Chain Reaction (PCR) were co-purified by "total DNA" binding resins in the presence of low concentrations (= 10^6 g^{-1}) of target DNA. In contrast, high concentrations of target DNA were readily purified by "total DNA" binding resins in a form that could be amplified by PCR. Based upon these results, the chemistry of a total DNA binding reagent was automated in a temperature-controlled renewable microcolumn. Technical issues that were overcome during protocol automation included the manipulation of non-spherical, silica microparticles; reagent/system incompatibilities; and buffer requirements and system programming compatible with on-line PCR. Significant effort has been devoted to the development of a flow-through, fluidically compatible PCR device, based upon the heating and fluidic principles encompassed in the PNNL renewable microcolumn technology. With the flow-through PCR module, the team successfully amplified 10^8 copies of 16S rDNA from 100 ng genomic DNA in ca. 45 minutes. More importantly, a successful decontamination protocol was developed that prevents DNA cross-contamination within the PCR module. Subsequently, a crude subsurface sediment extract was spiked with target DNA, purified on the automated system with a "total DNA" binding reagent, and the eluent amplified in the PNNL flow-through PCR module. This demonstration represents the first-ever successful automated nucleic acid extraction, purification, and amplification procedure and device specifically suited for environmental samples such as soils and sediments. Thus, the automated nucleic acid purification system and flow-through PCR module are ready for hardware and chemistry integration, in preparation for a flow-through Genometrix microarray detector.

37: *Peptide Nucleic Acid Arrays and Fluorescence Resonance Energy Transfer to Identify and Enumerate Microorganisms in Environmental Samples*

ID:	PNL97-11	
PI:	Darrell Chandler Environmental Microbiology Group	
Phone:	509 376-8644	
Partner:	PerSeptive Biosystems Framingham, MA	
FY99 Funding:		$250K
Total Project Funds:		$750K

Background

The detection and characterization of microorganisms in chemically complex environmental samples such as soil is currently limited by the lack of highly effective and automated methods for efficient chemical purification of cellular nucleic acids. This is especially important when the organisms of interest are present at low concentrations ($<10^4 g^{-1}$).

Research Objective

The objective of this project, conducted by Pacific Northwest National Laboratory and PerSeptive Biosystems, is to develop peptide nucleic acid (PNA) probes as affinity purification reagent**s** for the automated recovery and purification of nucleic acids (DNA and RNA) from crude environmental extracts. The project contributes to DOE's remediative missions by enabling the detection of specific bio- and/or pathogenic microorganisms in environmental samples such as soil, sediment, sludge, groundwater, wastewater, and aerosols.

Results

Studies focused on the mixed-phase hybridization characteristics of PNAs in crude environmental extracts and pure solutions relative to the behavior of a DNA oligonucleotide under identical solution conditions and within the context of automated nucleic acid sample preparation.

A significant relationship between total nucleic acid concentration and PNA probe efficacy was discovered, with implications for affinity purification of nucleic acids in low-biomass environmental samples. Bis-PNAs were investigated for their RNA binding and recovery properties in crude environmental extracts, representing the first use of PNA clamps as an RNA affinity purification reagent. Absolute recovery and detection limits for PNA, bis-PNA, and DNA affinity purification probes in sediment extracts were approximately 100-1000 copies of target DNA in 8.3 attomolar solutions. PNNL's temperature-controlled, renewable microcolumn technology was used to compare oligonucleotide and PNA probes coupled to a PerSeptive solid support. Both probes recovered 1 attamole of target in a competitive genomic background, comparable to benchtop procedures. Eight femtomolar concentrations of target were also purified/detected from crude aerosol samples, with 10-20% recovery efficiency and a 10 minute processing time. Unfortunately, PNA probes also co-purified polymerase chain reaction (PCR) contaminants, such that concentrated eluants inhibited the replication (PCR) process. Thus, novel surfaces and hybridization conditions will be required to utilize PNA probes for automated nucleic acid purification in these environmental samples. Cross-contamination was only evident when performing off-line PCR at single-copy sensitivity. An automated cleaning protocol was developed to remove residual contamination, but these solutions were incompatible with the renewable microcolumn materials. New flow-cells are now under construction and will be used to optimize automated PNA procedures.

38: *Rapid Prototyping for Bioceramics*

ID: ANL 95-08
PI: William Ellingson
Energy Technology Division
Phone: 630 252-5068
Partners: Zimmer, Inc.
Warsaw, IN
Midwest Orthopaedics
Chicago, IL

FY99 Funding: $42K
Total Project Funds: $900K

Background

Often times, accidents or necessary medical surgical procedures cause severe damage to the skeletal structure of humans. To replace the damaged skeletal structure usually means that either one of two methods is used: a bone from a cadaver is machined to fit the damaged bone, or a bone segment from someplace else on the person's body is removed and machined to fit. A new technology to produce artificial bone, referred to as rapid prototyping with bio-ceramics, will allow a damaged skeletal part to be repaired with a minimum of complications. The project transfers DOE funded research in ceramic materials to applications in human physiology.

Research Objective

This project between Argonne National Laboratory, Zimmer, and Midwest Orthopaedics is exploring the use of a new fabrication technology, Solid Freeform Fabrication (SFF), also commonly called Rapid Prototyping, to direct fabrication of bioceramic materials with a focus on reducing costs for bone segment replacements or small orthopedic implants. Two technology areas are being coupled together: reverse engineering using high resolution 3D x- ray computed tomographic imaging (commonly called CAT scans in medical applications), and the new SFF technology using bioceramics.

Recently, use of Tricalcium Phosphate (TCP) powder with new polymers has allowed the fabrication, debinding, and sintering of bioceramic orthopaedic implants which yielded sufficient properties for application. The fabrication was made possible by a new SFF feed system which allows improved delivery of the bioceramic powder/polymer mix. This high pressure extruder allows higher ceramic powder solids loading, thus reducing shrinkage. In addition, use of laser machining for the as-produced SFF bioceramics has also been demonstrated. The use of laser machining allows for a fast method to provide an appropriate surface finish. Extensive analysis of these materials is now in progress.

Publications and Presentations

1. S. Pekin, A. Zangvil and W. A. Ellingson, Proceedings of 1998 Solid Freeform Fabrication Conference, Austin, TX, submitted 1998.
2. S. Pekin, A. Zangvil and W. A. Ellingson, *Proceedings of the International Symposium on Advanced Materials with Biomedical Applications*, National Institute for Standards and Technology(NIST), Gaithersburg, MD, submitted 1999.
3. S. Pekin and A. Zangvil, Proceedings of the 1999 Solid Freeform fabrication Conference, Austin, TX, submitted 1999.

39: *Development of Tin-117m Stannic DTPA for the Therapy of Cancer in Bone*

ID:	BNL 99-10	
PI:	Suresh Srivastava Medical Department	
Phone:	516 344-4459	
Partner:	Diatide, Inc Londonderry, NH	
FY 99 Funding:		$125K
Total Project Funds:		$750K

Background

This year about 400,000 patients will develop bone cancer in the United States. Roughly one half of these will experience severe and chronic pain that may result in immobility and deterioration in quality of life due to side effects related to major narcotic treatments.

Research Objective

Brookhaven National Laboratory and Diatide, Inc. are conducting joint research on a new radiopharmceutical developed at BNL for treating cancer related bone pain. The goal of this project is to develop and test the application of a low-Diethylenetriamine-pentaacetic acid (DTPA) formulation of tin-117m stannic DTPA for the treatment in humans of primary osteoblastic osteosarcoma, and of bone metastases originating from this and other primary cancers. Prior research at BNL has shown that tin-117m provides relief from metastatic bone pain without the myelosuppressive effect associated with the other radiopharmaceuticals used for this purpose. Since tin-117m, as opposed to other comparable nuclides, can be administered in much larger therapeutic amounts before producing marrow toxicity, this project will develop its potential application for the treatment of cancer in bone.

The technical approach will include clinical trials in mice and dogs, and then in humans, to characterize and optimize the low-DTPA formulation. Animal studies will involve tissue biodistribution studies, pharmacokinetic measurements, dosimetry, mechanisms of localization in bone and other normal tissues, and determination of the maximum tolerated dose. A therapeutic trial will be performed in dogs with spontaneous osteosarcoma, using three dose levels (0.5, 1.0, and 2.0 mCi/kg) of tin-117m DTPA. In parallel, a low-dose (~0.5 mCi) Phase I study in patients to measure biodistribution and dosimetry will be undertaken. Based on therapeutic protocol and dose(s) found effective in dogs, Diatide, Inc. will modify the current GMP (good manufacturing process), carry out quality control assays, undertake acute and sub-acute toxicology studies, prepare the commercial IND (investigational new drug reporting), and conduct Phase I clinical trials. The project will eventually proceed to Phase II and III clinical trials and the preparation and submission of an NDA (new drug application) to the FDA for marketing approval. The project is an extension of the DOE's mission in the biological sciences to develop radio-pharmaceuticals as diagnostics and selective treatments for cancer.

40: *Development of a Non-Iodine-Based Radiographic Contrast Agent and a Complementary Monochromator for CT and Planar X-Ray Imaging Sources*

ID:	BNL99-09	
PI:	Avraham Dilmanian Medical Department	
Phone:	516 344-7696	
Partner:	Schering AG Berlin, Germany	
FY 99 Funding:		$125K
Total Project Funds:		$750K

Background

The worldwide cost of iodine agents used in radiographic measurements is about $3 billion dollars a year, and for new radiographic instruments (computed tomography (CT), angiography, and chest) is around $4 billion per year. In addition to costly operational expenses, the current state of the art suffers from three major problems. First, iodine-based contrast agents cause adverse reactions in substantial numbers of patients, including those with allergies, asthma, kidney diseases, and diabetes. These reactions can be severe or fatal. Second, iodine (Z=53) is not heavy enough to efficiently attenuate x rays at energies above 50 keV; Gd (Z=64), for example, is much better. Third, the broad-spectrum, filtered bremsstrahlung x-ray beams used are not ideal for contrast imaging because they have little intensity above the iodine's K-edge.

Research Objective

Brookhaven National Laboratory and Schering AG will develop a safe radiography contrast agent based on a lanthanide (Gd, Dy, or Yb), or Bi, using BNL's unique, monochromatic CT system Multiple Energy Computed Tomography (MECT) at the National Synchrotron Light Source (NSLS) in both CT cross sectional and planar modes (projections on a plate, film, or detector).

Animals and nonliving test subjects will be imaged with conventional systems at SUNY Stony Brook. MECT's monochromator and subject-positioning apparatus will be upgraded for this purpose. A high-throughput bent-crystal Laue monochromator will be developed to provide narrow-energy beams for planar radiography (e.g., angiography) and CT, using high-intensity rotating-anode tubes. A successful new contrast agent, combined with a narrow-bandwidth beam energy, should increase the image contrast-to-noise ratio by 3-fold or more. The monochromator will be tested with radiography and CT systems, and will then be used at Stony Brook to evaluate the compounds. Critical tasks will be: (1) BNL will upgrade the MECT system; (2) Schering AG will synthesize agents; (3) BNL will image the agents in phantoms, rabbits, and dogs using both MECT and conventional systems; and (4) BNL will construct a monochromator for planar radiography and CT, and use it at Stony Brook to test the compounds. Potential benefits include development of (1) a safer radiography contrast agent with enhanced imaging properties, and (2) a monochromator for planar radiography and CT. Finally, the project should lead to commercialization of a new contrast agent and imaging equipment. The work is an extension of the DOE's mission in life sciences to develop non-invasive diagnostics for biological dysfunction.

41: *Methods for Developing Monoclonal Antibodies that Recognize Protein Phosphorylation*

ID:	BNL98-01	
PI:	Carl Anderson Biology Department	
Phone:	516 344-3375	
Partner:	Oncogene Research Products Cambridge, MA	
FY 99 Funding:		$200K
Total Project Funds:		$607K

Background

One-third of all human cell proteins are phosphoproteins. Many of the protein activities in cells are regulated by reversible chemical modifications, the most frequent of which is phosphorylation. Detecting key protein modifications is often difficult. Researchers at Brookhaven National Laboratory have observed specific antibodies that recognize protein phosphorylation sites in eukaryotic cells. Such antibodies that recognize single or groups of phosphorylated sites have the potential to revolutionize molecular studies of eukaryotic cell regulation.

Research Objective

BNL and Oncogene Research Products are developing a facile method of making antibodies that recognize any of the many protein phosphorylation sites in eukaryotic cells with relative ease. The technique involves replacing the natural phosphate group with a chemically similar group (F_2Pab) that is not hydrolyzed by protein phosphatases. F_2Pab is chemically incorporated into the peptide as the Fmoc-derivative. The increased stability of F_2Pab peptide ensures that a higher fraction of the animal's immune cells will produce antibodies that recognize the phosphorylated protein.

Results

Critical tasks in this project include: (1) identifying a company that can synthesize the Fmoc-F_2Pab derivative required for preparing peptides: (2) synthesizing normal peptides, chemically phosphorylated peptides, and F_2Pab-derivative peptides corresponding to several known phosphorylation sites in p53, (3) immunizing rabbits and mice with the derivative compound, (4) purifying and evaluating the sera and hybridoma cell lines that are produced, and (5) developing assays that will measure the sensitivity and specificity of each antibody. Tasks (1)-(3) have been successfully performed. Oncogene Research Products is carrying out task (4) and is commercializing antibodies as stand alone reagents, and is exploring additional product formats, including development of quantitative assay kits. The methods and procedures developed should greatly improve the efficiency of generating the many new reagents that will be required in the future. Novel reagents based on single-chain antibody constructs may emerge from this work. The reagents developed by this project will be of direct benefit to studies designed to understand the consequences of low-dose exposures of human cells to DNA damage producing agents and for functional genomics. These studies are important aspects of DOE's missions to develop fundamental biological information and to advance technologies for use in research on the health effects of energy-related agents and processes.

42: *A Compact Scintillation Camera for Medical Imaging*

ID:	LBL99-14	
PI:	William Moses	
Phone:	510 486-4432	
Partner:	Capintec, Inc. Ramsey, NJ	
FY99 Funds:		$85K
Total Project Funds:		$750K

Background

Lawrence Berkeley National Laboratory and Capintec, Inc. are collaboratively developing a commercial line of compact nuclear medical imaging devices. LBNL has developed prototypes of several such devices based on scintillation crystal arrays coupled to photodiode arrays which are controlled with a custom integrated circuit. Capintec will incorporate these technologies into a line of commercial products directed at nuclear oncology and cardiology. The designs include a miniature imaging probe for inter-operative detection of radionuclides to assist in cancer surgery, a small compact camera for detection of thyroid disease, and two camera geometries appropriate for pre-surgical imaging of breast cancer and nodal metastases.

Research Objective

While the prototype devices demonstrated by LBNL have successfully proved the feasibility of the detector concepts, the exact physical form requires significant modification before it can be incorporated into commercially viable products. For example, the pixel sizes and number of pixels (which affect the photodiode array and the scintillator crystal array) must be modified, more robust readout electronics must be developed, and the electro-mechanical interconnections and packaging must be miniaturized and ruggedized. The LBNL role in the collaboration is to provide the expertise in the critical core technologies and further develop the readout electronics. Capintec will provide packaging design and technology, develop the requisite software, and convert the prototypes developed in this project into marketable products. The project supports DOE's development of nuclear medical imaging devices for screening and diagnosis of biological dysfunction.

43: *Development of Novel Biological Targeted Therapies for ErbB2 Oncogene Products*

ID:	LBL99-10
PI:	Ruth Lupu
Phone:	510 486-6874
Partner:	Coulter Pharmaceutical Palo Alto, CA
FY 99 Funding:	$90K
Total Funding:	$540K

Background

Each year approximately 1.5 million people in the U.S. are diagnosed with cancer, which can take many forms depending upon where it originates in the body. The disease is characterized by disruption of normal cellular control, by genetic mutation or defect, to excessive cell reproduction, resulting in the formation of a tumor. Tumors turn especially deadly when cancer cells metastasize to internal organs or spread throughout the body.

Research Objective

Lawrence Berkeley National Laboratory and Coulter Pharmaceutical are investigating the molecular and biological mechanism by which epithelial cells are converted to tumorigenic, invasive, and metastatic cancer cells. The observation that the growth factor heregulin (HRG stimulates cell growth) activates receptors, called erbB-2, erbB-3, and erbB-4, has allowed definition of a series of in vitro and in vivo models to investigate the role of HRG expression and the molecular basis of cancer. The goal of this project is to use these models to design novel targeted therapies for a variety of carcinomas which overexpress (overstimulate, causing abnormal cell growth) the erbB-2 oncogene product. To achieve this aim, a erbB-2 functional site has been defined. A previously characterized peptido-mimetic, corresponding to the predicted ligand/receptor interaction domain of the erbB-2 receptor extracellular domain, will be used.

The peptide interferes with ligand induction of receptor activation as well as with ligand-independent receptor activation. It has been shown that this peptido-mimetic, corresponding to the primary structure in erbB-2, blocks the anchorage-dependent and -independent growth of breast and prostate cancer cells overexpressing erbB-2. Furthermore, it was recently shown that the conjugated peptide induces a significant reduction in tumor growth of breast cancer cells in vivo in athymic nude mice. Studies at LBNL suggest that this peptide receptor mimetic provides a leading compound towards the development of a new therapeutic approach for malignancies which overexpress the erbB-2 oncogene product. The known peptide sequence will be used to develop peptide libraries containing all the possible sequences. Molecular diversity libraries represent a powerful new way to generate millions of assayable structures using only a minimum of preparative chemical steps. Solid phase synthetic techniques are used to prepare combinatorial peptide libraries on small resin beads, each having a unique sequence. The bead library can be passed through a biological assay whereby certain members can be identified as active and removed from the mass. Micro sequencing of the bead or beads will then yield the active peptide analog(s). In vitro and in vivo studies will be then performed to define the potential capacity of the peptides as therapeutic tools.

44: *A High Throughput Assay for Screening Novel Anti-Cancer Compounds*

ID:	LBL98-14	
PI:	Mina Bissell	
	Life Sciences Division	
Phone:	510 486-4365	
Partner:	Chiron Corporation	
	Emeryvlle, CA	
FY99 Funding:		$113K
Total Project Funds:		$700K

Background

Each year approximately 182,000 women in America develop breast cancer, and each year approximately 46,000 die from it. No other malignancy is as common among our nation's female population, and none more lethal to those between the ages of 40 and 45. The anxiety and fear generated by these statistics is intensified by the confusing and often conflicting reports from medical researchers. Almost half of all breast tumors are diagnosed in women who have none of the medical community's established risk factors. This lack of predictability is indicative of how much remains to be learned about the disease and its underlying causes. However, progress, is being made. There is at least one theory that has withstood the tests of time and scrutiny. The theory implies that there is a direct link between the development of breast cancer and a network of fibrous and globular proteins surrounding breast cells called the extracellular matrix, or ECM.

Research Objective

LBNL and Chiron, Inc. are using a novel tumor cell reversion model based on this observation, to develop a high-throughput assay, screen Chiron's combinatorial libraries of nearly a million compounds for activity in this assay, and characterize potential lead drugs for novel anti-cancer therapies. This project represents a qualitatively different strategic approach to standard molecular target-based cancer drug discovery. Chiron is one of only a handful of biotechnology companies that has succeeded in autonomously developing a drug and bringing it to market. The project is an extension of the DOE's investments in the life sciences and in structural biology.

Results

Research from the project has shown that the micro-environment in which the cell resides, and the cell's surface receptors, are dominant regulators of normal tissue function. It has been demonstrated that aberrations in the signals exchanged between the outside and inside of the cell can lead to epithelial cancers such as cancer of the breast and prostate. In a novel model system, it has been observed that manipulation of receptors outside of the tumor induces tumor cells to revert back to normal cell function.

Award

1. American Association for Cancer Research G. H. A. Clowes Memorial Award 1999.

Invention Disclosures

1. "Human AZ-1 Gene, Variants Thereof and Expressed Gene Products." M. Chen, M. Bissell, PVJBRef.: 2960.44 and 2960.44 PCT (HV)
2. "Isolation and Characterization of Breast Cancer Suppressor Candidate Genes MHFK1 and MHFK2", M. Chen, M. Bissell.

45: *Medical Accelerator Technology*

ID:	LBL94-36	
PI:	William Chu Accelerator and Fusion Division	
Phone:	510 486-7735	
Partner:	General Atomics San Diego, CA	
FY99 Funding:		$268K
Total Project Funds:		$1500K

Background

For more than four decades, under the auspices of DOE, LBNL has pioneered and developed technologies of treating human cancer using accelerated heavy charged particle (proton and heavier ion) beams. In 1991, the first hospital-based medical proton accelerator facility was built in Southern California. More than eight hospital-based facilities are being built worldwide by commercial firms. Although the first facility was built by a national laboratory, the subsequent facilities are being built as turn-key systems by the private sector.

Research Objective

Lawrence Berkeley National Laboratory and General Atomics (GA) of San Diego are cooperatively developing technologies to channel the extracted proton beam from the accelerator to the treatment room, and then deliver it accurately into the treatment volume in a patient. Specifically, the goals of the project are to develop beam transport systems to bring the protons to the treatment rooms' rotating gantries to aim the treatment beams precisely into patients from any angle, and patient positioners to align the patient accurately relative to the treatment beams. This project combines DOE-developed technology in high energy and nuclear physics to further missions in the life and medical sciences.

Results

At the Northeast Proton Therapy Center (NPTC) of the Massachusetts General Hospital in Boston, fabrication and installation is almost complete. The accelerator has been installed and successfully tested. In FY1998, LBNL and GA staff members collaborated in integrating the NPTC medical system for effective therapy delivery providing patient safety. Design and fabrication of the ion source and the low energy beam transport (LEBT) structure began in FY1999. Integrated testing of the ion source and LEBT will be performed in collaboration with GA staff members. Ion source and accelerator technologies will be transferred to GA for the manufacturing of commercial proton therapy tools. Specifically, a radiofrequency (RF) driven multicusp ion source for a 13.56 MHz operation with high proton percentage, will be designed. Computer simulations of ion beam extraction and LEBT systems have been performed. The new LEBT system will conform to the acceptance parameters of the Loma Linda type radiofrequency quadrupole (RFQ) injector with the proton beam accelerated to 35 keV. The ion source and LEBT system under development will be versatile and can be applied to different RFQ structures.

Publications

1. W. T. Chu, *Proc. of the Beam Instrumentation Workshop, Vancouver, 1994* (Ed. G. H. Mackenzie, B. Rawnsley, and J. Thomson), AIP Conference Proceedings 333, American Institute of Physics, New York, pp. 160-178 (1995).
2. W. T. Chu, *Nuclear Instruments and Methods in Physics Research* B99: 835 (1995).
3. W. T. Chu, *Ion Beam s in Tumor Therapy*, Chapman & Hall, pp. 234-245 (1995).
4. W. T. Chu, *Proc. of the 1995 Particle Accelerator Conference (PAC95), Dallas, TX, May 1-5,* 2394 (1995).
5. W.A. Barletta, W.T. Chu, and K.-N. Leung, *Review of Scientific Instruments* 69: 1085 (1998).
6. W. T. Chu, *Biomedical Uses of Radiation* (ed. W. R. Hendee), Wiley-VCH Publishers, Weinheim, New York, Chichester, Brisbane, Singapore and Toronto, pp. 1055 (1999).

46: *Development and Evaluation of Rhenium-188-Labeled Radioactive Stents for Restenosis Therapy*

ID:	ORL98-31
PI:	F. F. Knapp, Jr. Life Sciences Division
Phone:	423 574-6225
Partner:	InnerDyne, Inc. Sunnyvale, CA
FY99 Funding:	$206K
Total Project Funds:	$657K

Background

Over 400,000 coronary angioplasties are performed annually in the United States. Coronary artery disease occurs when cholesterol plaque builds up (atherosclerosis) in the walls of the arteries to the heart. While angioplasty is successful in opening coronary arteries in 90% of patients, about 40% of patients will develop recurrent narrowing at the site of balloon inflation.

Research Objective

Researchers at ORNL and InnerDyne are developing therapeutic radioisotopes for the inhibition of re-clogging of arteries (restenosis) following arterial balloon angioplasty. The objective of the project is the development of radiopharmaceuticals and their evaluation in animal models. For the restenosis research, methods have been developed for attachment of the rhenium-188 (^{188}Re) radioisotope to coronary "stents", which are platforms widely used by cardiologists serving as a platform to keep arteries open after angioplasty. Attaching the ^{188}Re radioisotope, which has ideal radionuclidic properties, and is readily available at relatively low cost, also offers a unique opportunity to deliver radiation.

Results

The effectiveness of using ^{188}Re-labeled stents to prevent restenosis have been demonstrated in preliminary swine studies. Animal studies are in progress and optimal coating technologies are being developed for stabilization of ^{188}Re. In addition, methods are being developed for the similar use of yttrium-90, another radioisotope with excellent properties for this application. The scope of these studies has been expanded to include the development of new cancer therapeutic sources using the palladium-103 (^{103}Pd) radioisotope. ^{103}Pd has previously been shown to be an excellent approach for the treatment of prostate cancer using implantable sources. The expanded scope of this research involves the design and chemical synthesis of new "bifunctional" chelates which can strongly attach ^{103}Pd and also be attached to biodegradable implantable sources for cancer therapy. The chemical synthesis of new ^{103}Pd chelates is being developed and the ^{103}Pd-labeled compounds will be prepared and their stability will be evaluated. This research supports DOE efforts to develop radioisotope technology in nuclear medicine, oncology, and other medical applications.

Publications

1. Zamora, P. O., Ferretti, J. A., Som, P., Choi, J., Kuan, P., Osaki, R., Stern, R., and Oster, Z. H., *J. Nucl. Med.*, 40, 183 (1999).
2. Kuan, H.M., Zamora, P.O., Som, P., Ferretti, J.A., Singletary, S., Choi, J., Pollack, W., Osaki, S., Stern, R., and Oster, Z.H., *Medical Physics*, 26, 1748 (1999).

47: *Interfacial Interactions of Biological Polymers with Model Surfaces*

ID:	PNL97-21	
PI:	Steven Goheen Materials and Chemical Sciences Division	
Phone:	509 376-3286	
Partner:	Ross Products Division Abbott Laboratories Columbus, OH	
FY99 Funding:		$257K
Total Project Funds:		$749K

Background

Enteral feeding tubes are devices which are used to gain access to the patient's gastrointestinal tract for the delivery of liquid nutritional products. Feeding tube clogging is one of the more significant problems associated with enteral tube feeding. The clogging is believed to be due to protein adsorption and the unfolding of these proteins on the tube surface. The time required to unclog these tubes, costs and patient intervention required to replace clogged tubes, and time a patient is unable to be fed as a result of a clogged tube can all be significant, and have provided the stimulus for research in this area. In addition, the costs attributed to this problem are borne by all medical providers, including the Federal government.

Research Objective

Protein adsorption and surface-mediated unfolding are not well enough understood to determine how to minimize clogging in feeding tubes. Joint research at Pacific Northwest National Laboratory and Abbott Labs should improve the understanding of that process so clogging can be prevented. The objective of the project is to use state-of-the-art methods to design, synthesize, and characterize surfaces for adsorption experiments. Additionally, new technologies to monitor the adsorption process are being developed.

Results

Molecular beam epitaxy, chemical vapor deposition, and self-assembling monolayer surfaces with controlled properties such as chemistry, topography, and heterogeneity have been constructed. The proteins fibrinogen and casein are being used in the adsorption experiments. These allow the study of two different protein sizes and chemistries. Quartz crystal microbalance, liquid chromatography/ mass spectroscopy, and atomic force microscopy are being employed to study adsorption in situ. Information on adsorption kinetics, isotherms, and protein conformation are being obtained in real time. Solid state nuclear magnetic resonance experiments have been conducted to identify specific protein residues that interact with the surface. This investigation has provided molecular level information on specific interactions that was not previously available. The researchers verified the binding of key proteins onto materials of interest to Ross Products. Also determined are conditions which promote and inhibit binding and unfolding of proteins on solid supports. The project is a unique interface of surface science and structural biology and supports DOE's basic research investments related to the studies of biological macromolecules.

Publications

1. S. C. Goheen and J. L. Hilsenbeck, *J. Chromatogr*. A, 816, 89 (1998).
2. J. Vincent Edwards, Sarah L. Batiste, Betty M. Gibbins, and Steven C. Goheen, *The Journal of Peptide Research*, accepted 1999.
3. J. Vincent Edwards, Sarah L. Batiste, Betty M. Gibbins, and Steven C. Goheen, *The Faseb J*. 13(7): A1495 (1999).
4. J. L. Hilsenbeck, B. M. Gibbins, and S. C. Goheen, *The Faseb J*. 13(7): A 1555 (1999).
5. S. C. Goheen, C. W. Herbold, J. H. Miller, J. G. Marx, and D. L. Springer, *The Faseb J*. 13(7): A 1495 (1999).
6. C. W. Herbold, S. C. Goheen, *J.Chromatography*, submitted 1999.

48: *Development of a High-Efficiency Rotary Magnetocaloric Refrigerator Prototype*

ID:	AL99-02	
PI:	K.A. Gschneidner, Jr. Metallurgy and Ceramics Division	
Phone:	515 294-7931	
Partner:	Astronautics Corporation of America Milwaukee, WI	
FY99 Funding:		$125K
Total Project Funds:		$750K

Background

Most commercial and residential refrigeration and air conditioner systems use ozone-depleting or global-warming volatile liquid refrigerants. Even the newest, most efficient units operate well below the maximum theoretical (Carnot) efficiency, and further improvements may be impossible with the existing vapor-cycle technology. Magnetic refrigerators are an environmentally sound alternative to vapor-cycle refrigerators and air conditioners. They use solid refrigerant(s) and common heat transfer fluids (e.g. water, water-alcohol solution, air, or helium gas) with no ozone-depleting and/or global-warming effects. Unlike the compression process of the vapor cycle, the magnetocaloric process has almost no dissipation, and therefore the magnetic refrigeration cycle has the potential for a very high efficiency.

Research Objective

The objective of this project, conducted by Ames Laboratory and Astronautics Corporation of America, is to build and test a rotary magnetic refrigerator prototype operating near room temperature. Three major tasks will be accomplished during the project: (1) the design, construction, and testing of a high-efficiency rotary magnetic refrigerator prototype, (2) the development of advanced magnetic refrigerants for use between -20 and +50 C, and (3) the modeling and simulation of permanent magnet arrays, which will provide the necessary field strengths for a rotary magnetic refrigerator without the need for a power supply. The project supports DOE's efforts to increase energy efficiency by reducing operating costs in air conditioning and refrigeration.

49: *Nonconsumable Metal Anodes for Primary Magnesium Production*

ID:	ANL98-05
PI:	Michael Pellin Materials Science and Chemistry Divisions
Phone:	630 252-3510
Partner:	Noranda Magnesium, Inc. Franklin, TN

FY99 Funding:	$220K
Total Project Funds:	$750K

Background

Magnesium has the highest strength to weight ratio of any structural metal. Led by rapidly increasing applications for light-weight, high performance materials, the global demand for magnesium is increasing prodigiously. However, the energy required for magnesium production is about one third the cost of the magnesium produced. This cost to product makes a cost effective alternative, to the present technology of using consumable carbon anodes for magnesium production, desirable. An alternate process, using nonconsumable metal anodes, will decrease materials and energy costs associated with magnesium production.

Research Objective

Noranda Magnesium Inc. is working with Argonne National Laboratory to develop a nonconsumable metal anode to replace consumable carbon anodes now used in commercial electrolysis cells for primary magnesium production. Research at ANL involves forming surface films on candidate metal alloys that are promising candidate materials, and investigation of these using surface analyses. Promising alloys are being tested as anodes in bench scale magnesium electrolytic cells. Alloys identified as optimal will be further bench tested by Noranda.

This project will provide the basis for developing a new class of corrosion-resistant materials, that can be used in harsh chemical environments, as nonconsumable anodes for magnesium production. The nonconsumable anodes will lower material and energy costs by direct anode replacement in currently operating electrowinning cells, eliminate emissions of CO_2 and per-fluorocarbons, and aid development of new energy-efficient cell designs, which will save up to 2 kWh per pound of magnesium. Argonne's improved understanding of the mechanisms associated with film formation on alloys, e.g., surface segregation and near surface diffusion, may provide the basis for developing a new class of corrosion-resistant materials. These materials support the DOE's initiatives to reduce energy use in the production of magnesium and aluminum.

50: *Advanced Separations Technology for Efficient and Economical Recovery and Purification of Hydrogen Peroxide*

ID:	ANL98-07	
PI:	Edward St. Martin Energy Systems Division	
Phone:	630 252-5784	
Partner:	United Technologies, Inc. Mt. Prospect, IL UOP Research center Des Plaines, IL	
FY 99 Funding:		$250K
Total Project Funds:		$750K

Background

Hydrogen peroxide is an important commodity chemical whose worldwide production exceeds 2 million tons per year. It is a very effective oxidant that is used in many chemical processes such as wood pulp bleaching and is environmentally friendly because it only produces water as a by-product. There are many other examples where the use of hydrogen peroxide in the manufacture of major oxygenated petrochemicals could lead to much simpler and environmentally benign processes. However, the current price of hydrogen peroxide is too high to make these alternative processes economical.

Research Objective

The project between Argonne National Laboratory, UOP, and United Technologies will develop new catalyst, chemical formulations and membrane separations technology that promise to significantly change the way hydrogen peroxide is manufactured and used. The objective of the project is to develop and commercialize this new technology for industrial production of hydrogen peroxide that is more efficient, economical, and safe.

Results

The overall concept for membrane separation of hydrogen peroxide has been demonstrated in the laboratory, and new oxidation resistant membranes are now being developed. Not only could this be a simpler and less expensive process, but it could also allow the development of new commercial applications and markets for hydrogen peroxide that are currently not competitive. For example, the technology could enable small-scale systems to be built on-site, thus enabling incremental increases in capacity and point-of-use plants. It is estimated that the overall production costs in a fully integrated process using this new technology could be 50% lower than the current process. The potential demand for these new applications would easily triple if not quadruple the current demand for hydrogen peroxide. Thus, hydrogen peroxide has the potential of being the ultimate "green" chemical if it can be manufactured more efficiently, economically, and safely than the current processes. This project supports DOE initiatives to promote industrial technologies which reduce the impact of waste intensive processes on the environment.

Patent

1. US Patent No. 5,662,878 E. St. Martin, 1999.

51: *Application of Oxygen-Enrichment Technology for Locomotive Diesel Engines*

ID:	ANL95-10	
PI:	Raj Sekar Energy Systems Division	
Phone:	630 252-5101	
Partners:	Association of American Railroads Pueblo, CO General Motors LaGrange, IL	
FY 99 Funding:		$10K
Total Project Funds:		$730K

Background

In 1996, highway diesels (light-duty vehicles, light-duty trucks, and heavy trucks) emitted 172,000 short tons of particulates under 10 micrometers in size, or 62.8% of the total, and 1.93 million tons of NO_x, or 27% of the total. Locomotives are also contributors: in 1990, 10% of all NO_x emissions from mobile sources were from locomotives, which released 980,000 metric tons of NO_x and 24,000 metric tons of particulate matter.

Resesarch Objective

Argonne National Laboratory and the Association of American Railroads are developing a technology that should allow diesel engines to operate more cleanly and efficiently. The goal of this project is to apply the oxygen-enriched combustion technology for locomotive diesel engines to achieve lower exhaust emissions and improved performance. The final objective of the project will be a demonstration of both oxygen-enrichment and NO_x catalyst technologies on a two-cylinder EMD 567B test engine, while using an air separation membrane in the engine intake and with an optimized lean NO_x catalyst in the exhaust.

Results

To make this technology a reality for locomotives, an air separation membrane and other associated auxiliary equipment will be connected at the engine air intake (after the air filter) to supply the desired oxygen-enriched combustion air. ANL is also collaborating with Compact Membrane Systems to develop a prototype air separation membrane for demonstration tests. While operating the membrane causes a parasitic power drain (the goal is < 3% of rated engine power), the increase in gross power could compensate these losses, resulting in a net gain in power and lower emissions for locomotives. The EPA's Tier 0 and Tier I emissions standards are primarily to reduce NO_x emissions from the current average level of 13.5 grams/brake-horsepower-hour to 7.4 and 5.5 respectively. Since the new oxygen-enrichment strategy alone can not provide such low NO_x levels, ANL collaborated with a catalyst manufacturer and developed a prototype NO_x catalyst for the test engine. Laboratory tests with the prototype NO_x catalyst indicate that engine-out NO_x is reduced by about 20 to 30% during the range of engine operating conditions. Tests are in progress to further improve the catalyst's NO_x reduction efficiency by injecting small quantities of diesel fuel in the exhaust. The project supports DOE's initiatives in carbon management to specifically reduce emissions from new generation vehicles. The project has resulted in publication of numerous journal and technical publications as well as the following awards and patents.

Award

1999 R&D 100 Award.

Patents

1. R.B. Poola, and R.R. Sekar, 1998, “Method and Apparatus for Reducing Particulates and NO_x Emissions from Diesel Engines Utilizing Oxygen Enriched Combustion Air,”
2. R.B. Poola, and R.R. Sekar, 1998, “Method to Reduce Diesel Engine Emissions-Part 1,”
3. R.B. Poola, and R.R. Sekar, 1998, “Method to Reduce Diesel Engine Emissions-Part 2,” 4.
   R.B. Poola, R.R. Sekar, and R.L. Cole, 1997, “Variable Oxygen/Nitrogen-Enriched Intake Air Systems for Internal Combustion Engine Applications,” United States Patent No. 5,649,517.

52: *Catalytic Production of Organic Chemicals Based on New Homogeneously Catalyzed Ionic Hydrogenation Technology*

ID:	BNL97-05
PI:	R. Morris Bullock Chemistry Department
Phone:	516 344-4315
Partner:	Dupont Wilmington, DE
FY 99 Funding:	$235K
Total Project Funds:	$705K

Background

Homogeneous transition metal-catalyzed hydrogenations are vitally important to the chemical industry, for diverse processes ranging from synthesis of high-volume commodity chemicals to small-scale, high-value pharmaceutical products. Dupont uses catalytic ketone hydrogenations in the synthesis of certain agricultural and pharmaceutical products.

Research Objective

Brookhaven National Laboratory and Dupont are developing new technology for the catalytic production of organic chemicals of commercial interest. The project is exploring the scope and selectivity of catalytic *ionic* hydrogenation technology, in which hydrogen is added to an organic chemical in the form of a proton followed by a hydride. Newly developed catalysts, which are different from numerous existing catalytic processes that rely on expensive precious metals such as rhodium, will enable the catalytic hydrogenation of ketones under remarkably mild conditions: room temperature and low pressure (3 atm) of hydrogen gas.

Results

A series of new homogeneous catalysts based on inexpensive and abundant metals, molybdenum and tungsten, was recently developed in this project. Studies, in which the phosphine ligand bonded to the metal catalyst was varied, indicate that sterically demanding phosphines generally give higher activity. Since the catalyst deactivation pathway appears to involve loss of phosphine, a new generation of catalysts is being explored which are anticipated to have a longer lifetime. Ionic hydrogenations also present the possibility of carrying out new selective transformations unattainable with traditional hydrogenation catalysts. These include the selective reductive dehydroxylation of polyols for the conversion of biomass-derived materials to fine chemicals as well as basic feedstocks. Dupont is also interested in using selective catalytic reductive dehydroxylation to convert polyols into diols, for use as polymer intermediates. These reactions may lead to useful commercial processes, and are also very attractive for environmental reasons, as they employ alternative-renewable feedstocks rather than petroleum-based feedstocks. This project extends DOE’s investments in basic energy research to initiatives in commodity and pharmaceutical products and in bioenergy.

53: *Optimized Catalysts for the Cracking of Heavier Petroleum Feedstocks*

ID:	LBL99-01	
PI:	Gabor Somorjai	
	Materials Sciences Division	
Phone:	510 486-4831	
Partner:	Catalytica, Inc.	
FY99 Funding:		$126K
Total Project Funds:		$650K

Background

Catalysts lower the energy required for chemical reactions to proceed and are widely used in petroleum refining and chemical manufacturing. The useful lifetime and, thus, the value of an industrial catalyst are limited by a process known as deactivation in which the efficiency of the catalyst declines over time. Understanding the deactivation process is essential for developing new catalysts with longer useful lifetimes.

Research Objective

Lawrence Livermore National Laboratory in collaboration with Catalytica, Inc will use a new surface science tool, ultraviolet (UV) Raman spectroscopy, to identify chemical species on the surfaces of catalysts *in-situ*, under actual reaction conditions. There are two industrially important catalytic systems under study at present. In the first study, zeolite-based catalysts are being developed to remove undesired sulfur compounds from gasoline. The goal of this project is to evaluate the mechanism by which sulfur is adsorbed on the catalyst. Of particular interest is the identification of catalyst "active sites" that actually interact with the sulfur. This is done by spectroscopically monitoring the identity of the surface species under reaction conditions. The second system under study is the "reforming" reactions of n- hexane and n-heptane with hydrogen that produce high octane gasoline by converting the reactants to benzene and toluene.

Deactivation in these catalysts proceeds via "coking", the buildup and polymerization of carbonaceous reaction byproducts on the surface of the catalyst. The vibrational spectra of these byproducts will be obtained by UV-Raman spectroscopy for identification purposes. Ultraviolet excitation is required in this case to avoid interference from black body radiation from the hot catalyst material. Identification of problematic surface species will allow determination of the precise mechanism by which deactivation occurs in this system. Information on catalyst reaction and deactivation mechanisms are useful to Catalytica in improving their catalysts. These improvements will have a major impact on the efficiency of petroleum refining and gasoline production. The new surface science tools under development will have applicability to general studies in catalysis and surface science and support the DOE's mission in design and characterization of advanced materials.

54: *An Air Conditioning System with Improved Efficiency for Hybrid/Electric Vehicles*

ID:	ORL95-09
PI:	Donald J. Adams Engineering Technology Division
Phone:	423 576-0260
Partners:	Nartron Corporation Reed City, MI Advanced Vehicle Systems, Inc. Chattanooga, TN Chattanooga Area Regional Transit Authority Chattanooga, TN Electric Transit Vehicle Institute Chattanooga, TN
FY 99 Funding:	$98K
Total Project Funds:	$670K

Background

Electric vehicles (EVs) are considered to be 97% cleaner than gasoline powered cars. Operation of a conventional car for a year produces 17 pounds of hydrocarbons, 14 pounds of nitrogen oxides, and 200 pounds of carbon monoxide. Unfortunately, range and cost remain major obstacles to selling electric vehicles. Batteries are very expensive and need to be replaced often. Even with breakthroughs in battery technology, power consuming functions such as lighting, power steering, breaking, and air conditioning act to dramatically reduce battery lifetime. Public and commercial fleet vehicles, such as buses, represent a viable target market for EV technology.

Research Objective

The primary goal of this project, between Oak Ridge National Laboratory and the partners, is to develop an advanced, highly efficient electric motor and controller for a mobile air conditioning compressor for an electric bus air conditioner system. To achieve this goal, the efficiency of the Nartron Corporation's high efficiency, microprocessor controlled, turbine driven, modular air conditioner will be improved, and the mass and size of the compressor motor will be reduced. The system will then be installed in an Advanced Vehicle System's electric bus that will be operated by the Chattanooga Area Regional Transit Authority. An air conditioning system with existing motor technology will be run on the same bus for comparison. This work supports DOE's mission in electric and hybrid electric vehicle development

Results

The electrical and mechanical design of an axial gap permanent magnet motor with challenging size and power constraints has been completed. The first prototype hardware including housing and assembly fixtures is complete. ORNL completed the stators and windings and a self-sensing controller and power inverter for the permanent magnet machine in FY 96. Activities in FY 98 concentrated on the supplier fabrication of the novel rotor and shaft sub-assembly, and Nartron's design and fabrication of the housing and assembly fixtures. Nartron procured the rotor and shaft sub-assembly in FY 99. Assembly is underway and will be followed by testing and evaluation prior to installation in a bus. A new motor controller with advanced soft-switching circuitry, developed at ORNL, promises to make electric and hybrid vehicles more practical. The 100-kilowatt inverter and controller, which are being tested aboard an electric bus in Chattanooga, TN represent breakthroughs in several areas, including cost, volume, weight, and reliability. The soft-switching circuitry helps reduce damaging power spikes and increases efficiency. Researchers plan to operate the system on a test track and city route and collect and evaluate data. A large number of publications, related to this project, have been published in peer reviewed journals.

Patents

1. J. S. Hsu, United States Patent No. 5,929,579, issued July 27,1999.
2. J. S. Hsu, D. J. Adams, United States Patent No. 5,914,552, issued June 22, 1999.
3. J. S. Hsu, United States Patent No. 5,886,445, issued March 23, 1999.

55: *Advanced Development of Desiccant-Based Air Conditioning Systems*

ID:	ORL95-06
PI:	James Sand Energy Division
Phone:	423 574-5819
Partner:	Fresh Air Solutions by Engelhard/ICC Hatboro, PA
FY 99 Funding:	$200K
Total Project Funds:	$640K

Background

Desiccants offer many advantages over conventional HVAC cooling systems, including: improved indoor air quality, reduced peak demand on summer peaking electrical utilities, utilization of waste heat, better humidity control, and reduced interior remodeling costs to replace building materials damaged by moisture and mildew. Specific benefits expected from mainstream application of desiccant systems in U.S. buildings are reductions in energy consumption by 0.1 quads annually by 2005 and by 0.4 quads in 2010: and reduction of carbon dioxide emissions by 6 million tons annually by 2005 and 24 million tons by 2010. Before desiccant systems can enter into broader markets, barriers to their wider acceptance must be addressed to make it easier for architects and building designers to select and apply these systems. Benchmark testing of desiccant systems under a wide variety of operating conditions is needed to provide an objective comparison of desiccant and conventional system performance and product maps that aid in equipment selection and application.

Research Objective

Oak Ridge National Laboratory and Fresh Air Solutions are developing the enabling technologies which will permit successful development of non-CFC (chlorinated fluorocarbons) commercial air conditioning systems. The goals of the project are to improve air quality in buildings, decrease commercial use of equipment that uses halogenated refrigerants and, reduce electrical energy consumption through the use of reactivated desiccant materials for dehumidification.

Results

ORNL has demonstrated a consistent set of “metrics” which can quickly and easily be used by heating, ventilation, and air conditioning engineers to rate and model the performance of desiccant components in air conditioning system designs. Several operating parameters, such as wheel speed, regeneration temperature, volumetric air-flow rate, wheel thickness, sector angles, and dessicant loadings, which affect the the ability of the desiccant to remove moisture, have been field tested. A number of performance parameters, which quantify the moisture removal process, such as latent capacity and latent coefficient of performance, have been defined. Successful mainstream market introduction and implementation of desiccant air conditioning technologies will reduce and operating costs in 21st Century buildings and significantly contribute to reduced atmospheric carbon emissions. This project complements DOE efforts to support research which accelerates adoption of new technologies for efficient energy use.

Publication

1. E. A. Vineyard, J. R. Sand, D. J. Durfee, *Am. Soc. Heat. Refridg. Aircond. Eng.*, submitted 1999.

56: *Direct Casting of Titanium Alloy Wire for Low-Cost Aerospace and Automotive Fasteners*

ID:	PNL99-02
PI:	Mark Smith Materials Sciences Department
Phone:	509 376-2847
Partner:	Dynamet Incorporated Albany Research Center (ARC) Washington, PA
FY99 Funding:	$125K
Total Project Funds:	$750K

Background

Titanium fasteners are used extensively in commercial and military aircraft applications due to their high specific strength, excellent corrosion resistance, and compatibility with composite materials. Titanium fasteners and coil springs are also being studied by the auto industry for use in PNGV (Partnership for a New Generation of Vehicles). Although the advantages provided by titanium are well established, the cost of producing the titanium wire/rod materials used in the manufacture of the fasteners is extraordinarily high. Current wire production methods require large ingots to undergo multiple reduction steps until a diameter of 7 mm or less is obtained. The reduction steps are energy intensive, require expensive equipment, and result in the generation of scrap materials and undesirable etchant and lubricant waste. Economic analysis indicates that direct casting of a titanium wire to a diameter slightly larger than the desired final product, followed by relatively small final reduction steps, will result in significant savings to the aerospace industry and other titanium wire/rod users.

Research Objective

Pacific Northwest National Laboratory and Dynamet will develop and optimize a core-wire direct casting technology for the production of titanium wire and rod products. The direct casting process involves the use of a titanium core wire to serve as the carrier substrate onto which titanium will be cast and solidified at high feed rates. The objectives of the project include the development of unique atmosphere-controlled casting equipment, the application of thermal models to optimize the design and operation of the casting process, and extensive materials testing and characterization to establish the capability of the process to match properties produced by conventional processing. The project extends DOE investments in materials characterization to develop process technologies which further reduction of industrial waste emissions.

57: *Highly Dispersed Solid Acid Catalysts on Mesoporous Silica*

ID:	PNL 97-28
PI:	Charles Peden Environmental Molecular Science Laboratory
Phone:	509 376-1689
Partner:	UOP Research Center Des Plaines, IL
FY99 Funding:	$125K
Total Project Funds:	$750K

Background

Homogeneous acid catalysts, such as sulfuric acid and aluminum chloride, are currently used to catalyze many industrially important reactions. Although these homogeneous acid catalysts are efficient, they are not environmentally benign and create many operational problems. These problems can be mitigated with solid acid catalysts. Tungstophosphoric acid and sulfated zirconia are two solid acid catalysts with super-acidity, yet both suffer from low catalytic efficiency. In addition, it is difficult to disperse tungstophorsphoric acid on supports due to its large cluster size, and sulfated zirconia generally suffers rapid deactivation. These problems can be minimized with the superior characteristics of mesoporous silica.

Research Objective

UOP Research Center and Pacific Northwest National Laboratory are jointly developing solid acid catalysts by coupling the advanced characteristics of mesoporous silica with the superacidic properties of tungstophosphoric acid and sulfated zirconia. The goal of the project is to exceed the performance characteristics of existing solid superacid catalysts, thereby enabling the chemical and petrochemical industries to replace homogeneous acid catalysts. Design and characterization of materials which impact energy efficiency and environmental acceptability supports DOE investments in materials science.

Results

To date, researchers have functionalized the surface of mesoporous silica for the dispersion of tungstophosphric acid and sulfated zirconia acid groups. PNNL has developed methods to graft tungstophos-phoric acid and to graft hydrous zirconia via *in-situ* hydrolysis. Highly dispersed solid acid catalysts with controlled loading density have been synthesized and characterized. These novel catalysts have been tested with two model reactions in the bench-scale testing unit at PNNL, i.e., alkylation of mesitylene by cyclohexene, and n-butane isomerization. The results indicate that highly dispersed Cs-tungstophosphoric acid catalysts show superior activity. It has also been shown that the activity of supported sulfated zirconia is highly dependent on factors such as the sulfation technique and catalyst pretreatment. Monolayer sulfated zirconia on mesoporous silica may not possess the superacidity that bulk sulfated zirconia does. In addition, UOP has obtained promising results with the supported Cs-tungstophosphoric acid catalysts using reactions of commercial importance, and is currently conducting further evaluation for their commercial applications.

Patent Pending

1. A Catalyst of a Salt That is Insoluble in a Polar Solvent on a Non-Metallic Porous Support and Method of Making, filed November 18, 1998.

Publications

1. P.D. Kaviratna, Y. Wang, A. Kim, Z. Nie and C.H.F. Peden, *Preprints of the Petroleum Division of the American Chemical Society* 43 295 (1998).
2. Y. Wang, A.Y. Kim, X.S. Li, L.Q. Wang, C.H.F. Peden, and B.C. Bunker, *American Chemical Society*, in press 1999.
3. Y.Wang, S.Choi, J.Liu, and C.H.F.Peden, *Catalysis Today*, in press 1999.

58: *Development of a New Generation Framework for Parallel Reservoir Simulation*

ID:	ANL-ACTI95-95
PI:	Tom Morgan Mathematics and Computer Science Division
Phone:	630 252-5218
Partners:	ARCO, BP Exploration, Chevron, Conoco, Cray Research, IBM, Texaco, Landmark Graphics, Mobil, Unocal, Scientific Software- Intercomp, Schlumberger - GeoQuest
FY99 Funding:	$215K
Total Project Funds:	$1184K

Background

The simulation of petroleum reservoirs is a vital component in the development of more efficient techniques for oil recovery. Current simulators are fundamentally limited in the size and complexity of the problems that they can handle. In addition, significant advances in geophysical, geological, and engineering measurements during the past ten years have resulted in huge increases in data and detailed description of oil and gas reservoirs. Ideally, all available information describing reservoir heterogeneity and a large number of important fluid and rock properties should be used in the simulations. However, most of this description data cannot be used with existing simulators.

Research Objective

The Argonne-ACTI partnership is leveraging many man-years of work and expertise of the collaborators in reservoir simulation, parallel numerical algorithms, and portable enabling technologies for parallel computing, to construct a prototype code, which will establish the foundation for general purpose parallel simulation. The design of the code will permit incorporation of several existing and emerging technologies of modern petroleum engineering.

Results

A number of significant accomplishments have been achieved to date by this project: (1) Development of a fully implicit equation-of-state 3D compositional model, general-purpose parallel adaptive simulator. (2) Incorporation of the linear solvers from the Portable, Extensible Toolkit for Scientific Computation (PETSc) package into the simulator. Simulator performance and scalability is largely dependent on the solvers. (3) Development of an object-based Fortran 90 framework to streamline the use of automatic differentiation. (4) Development of a multiblock domain decomposition approach for non-matching grids, multiple physical models, and multiple numerical schemes. (5) Excellent simulator performance on realistic problems demonstrated on IBM SP computers and clusters of PCs. The latter puts simulation within the economic reach of the smaller independent producers. (6) The same code can run on a full range of systems from a single workstation, a cluster, to the highest-end, highest-performance systems available. (7) The largest problem run to date: four million gridblocks and 32 million unknowns in approximately 23 minutes on a 128-processor IBM SP. The simulation of petroleum reservoirs is an important component of the DOE's mission to support the use of high performance computing for creation of a secure and economically viable domestic oil supply.

Publications

1. J. Abate, P. Wang, K. Sepehrnoori, and C. Dawson, *Communications in Numerical Methods in Engineering*, 15, 423 (1999).
2. S. Chippada, C. N. Dawson, M. L. Martinez, and M. F. Wheeler., Computer Methods in Applied Mechanics and Engineering Proceedings of the 1997 Symposium on Advances in Computational Mechanics, Vol. 151, pp. 105-129 (1998).
3. M.F. Wheeler and I. Yotov, Tenth International Conference on Domain Decomposition Methods, Contemporary Mathematics Vol. 218, J. Mandel et. al., eds, American Mathematical Society, 217 (1998).

Eight more papers have been accepted for publications in peer reviewed journals in 1999.

59: *Subsalt Imaging with Marine Magnetotellurics*

ID:	LBL-ACTI 95-90
PI:	Frank Morrison
Phone:	510 486-5080
Partners:	Scripps Institution of Oceanography, Amoco, BP, Chevron, Exxon, Geotools Corp., NWG Associates, Texaco, Unocal, Conoco
FY 99 Funding:	$177K
Total Project Funds:	$1050K

Background

Marine magnetotellurics (MT) is a new technique to augment seismic imaging in geological surveys. MT can reveal the size and thickness of underwater salt structures using differences in natural electromagnetic radiation in rock structures. Seismic imaging beneath high velocity, and often inhomogeneous formations, is a formidable task even with the most comprehensive 3-D surveying and processing techniques. However, the information can help researchers gauge the prospects for the sediment underlying the salt to be rich in oil or gas.

Research Objective

The objectives of the project are to (1) develop and test a seafloor MT system which is reliable and commercially feasible; (2) demonstrate the resolution of 3-D marine MT to the petroleum industry in the Gulf of Mexico; (3) develop new MT interpretation software capable of providing the necessary interpretation capabilities for petroleum exploration; (4) develop new joint inversion algorithms which will integrate all available seismic, gravity, and electrical data in producing a common unified earth model; and (5) move the technology for MT to commercialization.

Results

The first three of the above objectives have been achieved. A successful field trial was conducted in the Gulf of Mexico in the summer of 1998. This survey produced additional data which will be used to validate the MT software interpretation of 3D structure. The single remaining technical objective, which the oil industry sponsors consider extremely important, is the development of a joint inversion package which allows the MT interpretation software to integrate quantitatively all the available seismic, gravity, and electrical data (from MT) in a common geological model. This joint inversion requires the development of a mathematical formulation of the problem, building of new computer algorithms, and development of a software interface to permit the interpreter to move the different data sets into a common inversion environment. In the last year, a new gravity inverse algorithm which is robust and suitable for incorporation into a joint MT-gravity-seismic inverse was developed. The prototype joint MT-gravity inverse algorithm is currently under test. The project supports the DOE's commitments in high performance computing to enhance, apply, and transfer advanced computational technology for finding, developing, and producing natural gas and oil.

60: *Optimal Fluid Injection Policy and Producibility in Fractured, Low Permeability Reservoirs*

ID:	LBL-ACTI 95-92	
PI:	Tad Patzek Earth Sciences Division	
Phone:	510 643-5834	
Partner:	Aera Energy Bakersfield, CA	
FY99 Funding:		$128K
Total Project Funds:		$750K

Background

One of the oil industry's most perplexing problems is the inability of current production processes to coax to the surface nearly two-thirds of the oil in a typical reservoir. More than 350 billion barrels of crude oil discovered in the United States - twice the amount that has been produced - fall into this "unrecoverable" category, and almost 45 percent of this oil has already been permanently abandoned. The design and operation of wells and enhanced oil recovery systems require an accurate assessment of fractures and other well features. Improved prediction methods on reservoir flow characteristics will enhance the accuracy of the computer simulations used to develop more efficient oil recovery processes.

Research Objective

LBNL is working with the Berkeley Sensor and Actuator Center at Aera Energy and Integrated Micro Instruments to apply combined microsensor and computer technology which will change the paradigm of field-wide control of oil and gas recovery operations. The goal of the research is to produce a fully integrated, supervisory control system of oilfield injection projects using vast arrays of very cheap, smart sensors linked to parallel computers. The development of the Computer-Assisted-Operations software tools and microsensors to promote higher, cheaper, and safer recovery from fractured, low-permeability oilfields supports the DOE's initiatives in advanced computational technology.

Results

A number of observations have been modeled, with the following results: (1) hydrofracture extension during water and steam injection is inevitable and can be catastrophic at times; (2) fluid flow is almost perpendicular to the growing fracture and can be approximated by a 1D model; and (3) the average rate of fracture growth can be predicted from early injection data. An optimal process-based injection controller has been designed. It has been demonstrated that the optimal injection pressure depends not only on the instantaneous measurements, but also on the whole history of the injection and of the fracture area growth. A graphical controller software in C++ has been written. A procedure has been devised that allows estimation of the hydrofracture size. Unique surveillance software has been developed for waterflood operations. The software communicates dynamically with any structured query language database that stores the field data, giving automatic network access to the most current field information. The software allows both static and temporal visualization and analysis of the existing field data, either on a well-by-well basis or on a field-wise basis. The software analyzes the nearest-neighbor interactions between producers and water injectors; waterflood response; and growth of injection hydrofractures. It forecasts production.

Publications

1. Vegas-Landeau, M. A., R. Propp, P. Colella, T. W. Patzek, SPE 38457, *SPEJ*, 200-209, 1998.
2. Zwahlen, E. and T. W. Patzek, *In Situ*, 21(4), 297, 1997.
3. Patzek, T. W. and A. De, *Int. J. Petr. Eng.*, accepted 1999.
4. Patzek, T.W., and D. B. Silin, *Transport in Porous Media*, submitted 1999.
5. Silin, D. B., Patzek, T.W., *Transport in Porous Media*, submitted 1999.
6. Nikravesh, M., A. R. Kovscek and T. W. Patzek, in the Proceedings of the 1996 Biennial Conference of the North American Fuzzy Information Processing Society - NAFIPS, M. H. Smith, M. E. Lee, J. Keller, J. Yen Editors, pp. 164-170, Berkeley, CA, June 19-22, 1996.

59: *Subsalt Imaging with Marine Magnetotellurics*

ID:	LBL-ACTI 95-90
PI:	Frank Morrison
Phone:	510 486-5080
Partners:	Scripps Institution of Oceanography, Amoco, BP, Chevron, Exxon, Geotools Corp., NWG Associates, Texaco, Unocal, Conoco
FY 99 Funding:	$177K
Total Project Funds:	$1050K

Background

Marine magnetotellurics (MT) is a new technique to augment seismic imaging in geological surveys. MT can reveal the size and thickness of underwater salt structures using differences in natural electromagnetic radiation in rock structures. Seismic imaging beneath high velocity, and often inhomogeneous formations, is a formidable task even with the most comprehensive 3-D surveying and processing techniques. However, the information can help researchers gauge the prospects for the sediment underlying the salt to be rich in oil or gas.

Research Objective

The objectives of the project are to (1) develop and test a seafloor MT system which is reliable and commercially feasible; (2) demonstrate the resolution of 3-D marine MT to the petroleum industry in the Gulf of Mexico; (3) develop new MT interpretation software capable of providing the necessary interpretation capabilities for petroleum exploration; (4) develop new joint inversion algorithms which will integrate all available seismic, gravity, and electrical data in producing a common unified earth model; and (5) move the technology for MT to commercialization.

Results

The first three of the above objectives have been achieved. A successful field trial was conducted in the Gulf of Mexico in the summer of 1998. This survey produced additional data which will be used to validate the MT software interpretation of 3D structure. The single remaining technical objective, which the oil industry sponsors consider extremely important, is the development of a joint inversion package which allows the MT interpretation software to integrate quantitatively all the available seismic, gravity, and electrical data (from MT) in a common geological model. This joint inversion requires the development of a mathematical formulation of the problem, building of new computer algorithms, and development of a software interface to permit the interpreter to move the different data sets into a common inversion environment. In the last year, a new gravity inverse algorithm which is robust and suitable for incorporation into a joint MT-gravity-seismic inverse was developed. The prototype joint MT-gravity inverse algorithm is currently under test. The project supports the DOE's commitments in high performance computing to enhance, apply, and transfer advanced computational technology for finding, developing, and producing natural gas and oil.

60: *Optimal Fluid Injection Policy and Producibility in Fractured, Low Permeability Reservoirs*

ID:	LBL-ACTI 95-92	
PI:	Tad Patzek Earth Sciences Division	
Phone:	510 643-5834	
Partner:	Aera Energy Bakersfield, CA	
FY99 Funding:		$128K
Total Project Funds:		$750K

Background

One of the oil industry's most perplexing problems is the inability of current production processes to coax to the surface nearly two-thirds of the oil in a typical reservoir. More than 350 billion barrels of crude oil discovered in the United States - twice the amount that has been produced - fall into this "unrecoverable" category, and almost 45 percent of this oil has already been permanently abandoned. The design and operation of wells and enhanced oil recovery systems require an accurate assessment of fractures and other well features. Improved prediction methods on reservoir flow characteristics will enhance the accuracy of the computer simulations used to develop more efficient oil recovery processes.

Research Objective

LBNL is working with the Berkeley Sensor and Actuator Center at Aera Energy and Integrated Micro Instruments to apply combined microsensor and computer technology which will change the paradigm of field-wide control of oil and gas recovery operations. The goal of the research is to produce a fully integrated, supervisory control system of oilfield injection projects using vast arrays of very cheap, smart sensors linked to parallel computers. The development of the Computer-Assisted-Operations software tools and microsensors to promote higher, cheaper, and safer recovery from fractured, low-permeability oilfields supports the DOE's initiatives in advanced computational technology.

Results

A number of observations have been modeled, with the following results: (1) hydrofracture extension during water and steam injection is inevitable and can be catastrophic at times; (2) fluid flow is almost perpendicular to the growing fracture and can be approximated by a 1D model; and (3) the average rate of fracture growth can be predicted from early injection data. An optimal process-based injection controller has been designed. It has been demonstrated that the optimal injection pressure depends not only on the instantaneous measurements, but also on the whole history of the injection and of the fracture area growth. A graphical controller software in C++ has been written. A procedure has been devised that allows estimation of the hydrofracture size. Unique surveillance software has been developed for waterflood operations. The software communicates dynamically with any structured query language database that stores the field data, giving automatic network access to the most current field information. The software allows both static and temporal visualization and analysis of the existing field data, either on a well-by-well basis or on a field-wise basis. The software analyzes the nearest-neighbor interactions between producers and water injectors; waterflood response; and growth of injection hydrofractures. It forecasts production.

Publications

1. Vegas-Landeau, M. A., R. Propp, P. Colella, T. W. Patzek, SPE 38457, *SPEJ*, 200-209, 1998.
2. Zwahlen, E. and T. W. Patzek, *In Situ*, 21(4), 297, 1997.
3. Patzek, T. W. and A. De, *Int. J. Petr. Eng.*, accepted 1999.
4. Patzek, T.W., and D. B. Silin, *Transport in Porous Media*, submitted 1999.
5. Silin, D. B., Patzek, T.W., *Transport in Porous Media*, submitted 1999.
6. Nikravesh, M., A. R. Kovscek and T. W. Patzek, in the Proceedings of the 1996 Biennial Conference of the North American Fuzzy Information Processing Society - NAFIPS, M. H. Smith, M. E. Lee, J. Keller, J. Yen Editors, pp. 164-170, Berkeley, CA, June 19-22, 1996.

61: *Advanced Computational Analysis of Drill Cuttings for Real-Time Well Site Decisions*

ID:	LBL-ACTI 95-94
PI:	Larry Myer
Phone:	510 486-6456
Partner:	Terra Tek, Burlington Resources, Union Pacific Resource, BP-America, ARCO, E&P Technology
FY 99 Funding:	$180K
Total Project Funds:	$2955K

Background

The engineer on a drill rig platform possesses limited information about the properties of the subsurface being drilled thousands of feet below. Nonetheless, critical decisions must be made "on-the-spot" with regard to the stability of the well and the location and quality of reservoir rock. This project focuses on development of a new technology utilizing rock fragments produced during drilling to provide the information on rock properties needed to make these rig-site decisions. The successful implementation of this technology is estimated to yield at least 300 million barrels of oil equivalent. as bypassed producing zones are developed, and missed opportunities are reduced. Improving the capability of the Nation's petroleum industry to increase the supply of secure, domestic oil is a core mission of the DOE's initiatives in supercomputing and fossil energy.

Research Objective

This project combines a unique mathematical modeling capability developed at LBNL with exploration experience and expertise of the industry partners to develop efficient computational models which will be used to calculate flow properties including permeability, capillary pressure, relative permeability, and mechanical properties based on images of the rock pore space derived from cuttings. This direct calculation takes into account the effect of microscale heterogeneity, thereby mitigating one of the major sources of uncertainty in currently available analysis methods. Highly efficient computational models for flow are made possible by innovative application of graph theory, an established branch of topology. Other simple, inexpensive, direct, and indirect measurements of drill cutting properties, which are available or under development, will be combined with the algorithms developed in this project.

Results

Key milestones for the project have been met. These include development of a first generation graph theory based computer model, called GAPPFEM, for calculation of flow properties and validation of the model with laboratory measurements. Current efforts are directed toward implementation of a new "front-end" which allows direct conversion of a high resolution image into a network for calculation of flow properties.

Publications

1. Huang, P., Yang, G., Myer, L., Cook, N., and Witherspoon, P., *International Journal of Rock Mechanics & Mining Science*, Vol 34, No.3-4, Paper No. 135, Proceedings of 36th U.S. Rock Mechanics Symposium, 1997.
2. Huang, P., Myer, L., and Yang, G., *Proceedings of 9th International Congress on Rock Mechanics*, Paris, Balkem (publisher), 1999.
3. GAPPFEM, Graph Analysis Program Package for Flow in Earth Materials, G. Yang,- a graph theory based network simulator for calculation of multiphase flow properties of reservoir rock.

62: *Electrodialysis for Salt Recovery and Reuse*

ID:	ANL-AMTEX2
PI:	Shih-Perng Tsai Energy Systems Division
Phone:	630 252-5006
Partner:	Institute of Textile Technology Spartanburg, SC
FY99 Funding:	$160K

Background

The U.S. textile industry uses 800 million lb/yr of sodium chloride and sodium sulfate, mostly in dyeing processes. These salts are not consumed during the processes and remain in dyebath effluents. A typical dyeing and finishing plant discharges about 20 million lb/yr of salts. This results in the loss of the salt value and high costs in environmental compliance. Thus, there is a significant opportunity to apply efficient and cost-effective separation technologies to recover the salts for reuse.

Research Objective

The goal of this project, conducted by Argonne National Laboratory and the Institute of Textile Technology, is to develop electrodialysis processes for the recovery and reuse of salts from dyebath effluents. Argonne has developed an electrodialysis process for the recovery of salts from dyebath effluents. Electrodialysis uses selective permeability of ion-exchange membranes to purify and concentrate ionized species from aqueous streams. In this process, the salt present in the dyebath effluents is separated from unused dyes and other chemicals, and a brine solution is generated for reuse in making new dyebaths. This enables reuse of salt, lowers a textile plant's operating costs, and eliminates an unwanted discharge into the environment.

Results

Laboratory scale electrodialysis experiments have been conducted since 1994 with simulated and actual dyebath effluents. Process feasibility was demonstrated, and suitable technical parameters and process conditions were established in laboratory-scale experiments. The thrust of the work has been a pilot-scale field demonstration which was successfully completed in a textile mill in 1999. In this field demonstration, salt was recovered from several dyebath effluents using different process schemes. The process performance, in terms of the salt flax, energy consumption, and brine quality, was better than or comparable to the previous laboratory results. The recovered brine, which has a high concentration of salt but no detectable color, is being evaluated by the industry partners for reuse. The electrodialysis technologies being applied to the textile industry for salt recovery have applications in other processing industries for pollution prevention and efficient product separation. These technologies will increase the competitiveness of the textile industry while reducing the environmental impact of its operation and are thus compliant with the mission of DOE sponsored programs for the chemical, agriprocessing, and forest products industries. The electrodialysis technologies also support the DOE's environmental remediation and restoration programs. Publications resulting from work on this project have been withheld due to proprietary interests of the CRADA partners.

63: *Demand Activated Manufacturing Architecture (DAMA) Low Cost Apparel System (LCAS)*

ID:	ORL-AMTEX 1
PI:	Bill Grimmell Computer Science and Mathematics Division
Phone:	423 574-6162
Partner:	Institute of Textile Technology Charlottesville, VA
FY99 Funding:	$500K

Background

The LCAS work was motivated by a DAMA small and medium size apparel company study. This study uncovered a need for a low cost capability for the integration of PC based, poorly documented, software packages (used by most of these companies) with each other and with trading partner communication packages, including those providing traditional Electronic Data Interchange (EDI). A preferred approach to meeting this need would involve a procedure analogous to systems identification and (full or partial) automatic code generation which could be implemented through a significant extension of previous work done at ORNL. DAMA supports the DOE objective of improving the performance of the US textile industry and thereby enhancing competitiveness.

Research Objective

The objective of this project between ORNL and the Institute of Textile Technology is to develop a design and prototypes of an integration platform and tool set to provide a relatively quick means for integrating the classes of software packages that the target companies currently use and are likely to use in the near future. The approach is to provide a modularized highly general and generic "package integration module" (PIM) with specific modules and/or parameter tables for each set of software packages that is to be interfaced in any particular installation. Traditionally, EDI utilizes a server provided by an outside value added network. The tool set will allow identification of the impact of software package user interface operations on the package's internal database. The output of this tool set will then provide input to the code generation software to generate the PIM software module that is specific to a particular software package. The approach will also be amenable to persons with only modest computer knowledge. A pilot version of the system will be engaged in 2000.

Results

Two prototypes in which an apparel manufacturing software package, a "VAN" EDI software package, and an ORNL "direct Internet" communication package were integrated via versions of the PIM have been developed along with an early version of the tool set. A preliminary methodology that can be used for representing software package database modifications as a result of the types of input expected has been outlined. The representation is aimed at producing a suitable format for input to the code generation software. The ORNL communication package provides secure EDI and other communication without use of a VAN. It provides two modes of communication, a primary mode of direct internet communication between trading partners and a secondary email mode.

64: *Computer-Aided Fabric Evaluation (CAFÉ)*

ID:	ORL-AMTEX6
PI:	Glenn Allgood Instrumentation and Controls Division
Phone:	423 574-5673
Partner:	Institute of Textile Technology Spartanburg, SC
FY99 Funding:	$405K

Background

The U.S. textile industry has been under market pressure, from offshore competition, to reduce product costs and enhance product quality. Technology innovations that increase process efficiency, i.e., technologies that meet stringent economic and functional requirements, are capable of streamlining operational costs and thus will increase the competitiveness of US industry.

Research Objective

Oak Ridge National Laboratory, in collaboration with the Institute of Textile Technology and their AMTEX partners, are developing systems, methods, and approaches that inspect cloth for structure and optical flaws and provide process information as it relates to the construction. These requirements dictate that inspection and analysis be performed close to the point of fabric formation, i.e., on-loom and in the print lay-down area. In addition to this, Computer-Aided Fabric Evaluation (CAFÉ) will develop a machine diagnostic capability to identify and quantify machine problems that contribute to product off-quality. The project extends DOE basic research investments to field-proven sensor and imaging systems development, and also furthers computational research through development of pattern recognition algorithms useful in national defense and security.

Results

The project has developed and delivered to the CAFÉ industry partners four specific technological innovations. The first is the CAFÉ Economic Model, which has been used to determine the economic viability of CAFÉ technologies and the total impact on the manufacturing infrastructure. It is being considered for copyright. Technologies that have been developed to support fabric and color inspection includes a Pick Measurement Device and an Imaging Colorimetry System. The Pick Measurement Device is a laser-based system that provides information about fabric construction (density, total picks, and process information). The first generation system was delivered in 1996. A beta version was delivered in 1998 for compliance testing and is currently undergoing algorithm modifications to allow detection and qualification of fabric anomalies. The proof-of-concept Colorimetry System was also successfully delivered in 1998. The system provides a novel color transform algorithm based on the Projection on Convex Surfaces (POCS) algorithm. Current efforts include enhancements to the algorithm (including segmentation) and upgrades to the hardware and firmware. The system is slated for a comprehensive compliance test and hand-off to ITT and its color vendor. An invention disclosure is being filed on the system. Machine Diagnostics are slated for completion in FY99 with a deployment of the system into Y12's production facility. The current deployment target is a major ventilation system.

Publications

1. Final Report for CRADA Number ORNL94-0253 "The AMTEX Computer-Aided Fabric Evaluation (CAFE) Project." Report number C/ORNL94-0253
2. Other CAFE publications are CRADA protected.

Patent

1. 1998 U.S. Patent No.5,825,501, D. K. Mee, G. O. Allgood, J. C. Turner, D. A. Treece, L R. Mooney, M. G. Duncan.

65: *Technology Resource Conservation (TReC) Environmental Decision Tools*

ID:	PNL-AMTEX1
PI:	Tapio Kuusine EnvironmentalTechnology Division 509 372-4234
Partner:	Institute of Textile Technology Charlottesville, VA
FY99 Funding:	$370K

Background

To be competitive in the international marketplace, textile manufacturers must produce superior products that are delivered on time and produced with minimum cost and liability. Unfortunately, many of the largest opportunity costs are hidden, as they have been incorporated into operating standards or exist due to historical industry practices. Many of these hidden costs in the textile chain are in the environmental and energy areas. Advanced decision systems, or tools, are increasingly important as business and environmental decisions become more complex and interrelated.

Research Objective

The objective of this project is to provide an opportunity for textile companies to more thoroughly evaluate the environmental and cost consequences of business decisions. This is being done by using environmental decision tools, developed by Pacific Northwest National Laboratory in conjunction with the Institute of Textile Technology (ITT) and their AMTEX partners. These capabilities will further DOE's core missions of reducing industrial energy consumption and pollution.

Results

Textile environmental decision tool development was initiated at PNNL in FY95. Two prototype software products were developed: LC Advantage and the Pollution Prevention Design Guidelines for Engineers (P2EDGE) Model. LC is an analytical tool that allows a product or process designer to understand the economic and life-cycle environmental consequences of design alternatives. P2EDGE-Textile helps industrial product and process designers identify pollution prevention opportunities within their company and plants. Work also has been initiated on a third TReC environmental decision tool product, a prototype software application called Color Advantage, that will allow users to incorporate environmental considerations into the selection of textile colorant systems. Additionally, a fourth and final TReC environmental decision tool software product called Chem Advantage, built largely on the same shell as Color Advantage, will allow users to make comparisons among alternative chemical products and evaluate pollution prevention priorities based on chemical inventories and available substitutes.

Award

1. 1998 R&D100 Award.

Publication

1. Kuusinen, Tapio L., Robert Barker, and Donald Alexander, Technical Association of the Pulp and Paper Industry, Nonwovens Division Annual Meeting, Memphis, Tennessee, March 17, 1997. *TAPPI Journal*, Vol. 81, No. 3, 179, 1998.

66: *Carbon Dioxide Based Sizing and Desizing*

ID:	PNL-AMTEX3
PI:	Larry Bowman
Phone:	509 376-1066
Partner:	Institute of Textile Technology (ITT) Charlottesville, VA
FY 99 Funding:	$565K

Background

Conventional methods for textile sizing and desizing (also know as slashing) consume a large amount of energy and generate a significant volume of waste water. Prior to weaving, size is added to yarn using a water solution, and the yarn is then dried before it is woven. Desizing of the woven fabric generates a large volume of waste water containing the spent size material.

Research Objective

Pacific Northwest National Laboratory, in conjunction with the AMTEX partners, is developing a new sizing and desizing technology that consumes much less energy and generates virtually no waste. The objective of the project is to develop sizing and desizing methods that allow materials to be used for weaving cotton/polyester blends and then be recovered and reused. This goal furthers DOE missions to access modern textile manufacturing processes which discharge zero net waste to the environment.

Results

PNNL has developed a new class of size materials that are soluble in supercritical or liquid carbon dioxide. In a small weaving trial at ITT, these size materials provided equivalent or superior abrasion resistance compared with conventional size. Two sizing/desizing application methods have been investigated: electrostatically-assisted deposition of powdered size and immersion in a solution of size in liquid carbon dioxide. Demonstration systems for both methods were developed in FY 98 and tested in FY 99. PNNL sized a small warp by each method, and ITT is conducting weaving trials. PNNL will also desize the woven fabric using liquid carbon dioxide.

Publications

1. L. E. Bowman, C.G.Caley, R.T. Hallen, and J. L. Fulton, *Textile Research Journal*, Vol 66, No. 12 (1996).
2. L. E. Bowman, N. H. Reade, R. T. Hallen, A. Butenhoff, Textile Research Journal, Vol 68, No. 10 (1998).

Patent

1. J. L. Fulton, C. R. Yonker, R. T. Hallen, E.G. Baker, L. E. Bowman, L. J. Silva. "Method for Sizing and Desizing Yarns with Liquid and Supercritical Carbon Dioxide Solvent" U.S. Patent 5,863,298, 1999.

Invention Reports

1.E-1700 "In-Situ Extraction of Initiator" filed with IPS on July 27, 1998.
2.E-1775 "Polymer Purification" filed with IPS on April 22, 1999.

67: *Optimization of Binding Agents in the Solidification/Stabilization of Swarf Materials*

ID:	ANLRAP 99-100
PI:	Robert Peters Energy Systems Division
Phone:	630 252-7773
Partner:	Solvent Systems International, Inc. Lake Bluff, IL

FY 99 Funding:	$5K
Total Project Funds:	$5K

Background

There are more than 100,000 facilities in the primary metals industries or the fabricated metal products industry which generate swarf from machining, polishing, grinding, and honing operations. Automobile industries and machine-tool industries are major producers of this waste. The metal fines are mixed with machining oils and lubricants. Metal fines are pyrophoric (spontaneously igniting), and large dumps of these fines tend to catch fire. Although landfills accept these wastes, landfill owners recognize that these are undesirable wastes, due to their tendencies to rapidly oxidize and create hot spot flare-ups (fires). At present, there is no cost-effective method to recycle swarfs. These waste materials often contain ~60 wt.% recyclable metal. These fines need to be solidified so that they can be fed into blast or arc furnaces for recycle and reuse.

Research Objective

The purpose of this project is to develop an agglomeration process to convert fine particulate metals (swarfs) into a form suitable for recycling such as forming dense, hard recyclable forms. To accomplish the overall objective, the following tasks have been undertaken: (1) characterization of several swarfs; (2) additive (binder) optimization studies; and (3) production of "optimized" bricks.

Results

Preliminary results include the identification of an appropriate binder, a phosphate-based material that can solidify representative waste streams collected from companies such as General Motors and Scot Industries. A waste loading of 80% to 90% has been achieved. Solidified products had compressive strengths exceeding 2,000 psi. Apparent bulk densities of the samples exceeded 2.2 g/cm^3. Drop tests to simulate their survival in rough handling during transportation and feeding in furnaces showed that the solidified products had good impact resistance and structural integrity. Although the process has not been fully optimized, rough cost evaluations show that the binder costs can be as low as ~$30/ton of waste, while the market price for the solidified waste forms can from $50 to $70/ton. Thus the process can be cost effective.

68: *Decontamination of Stainless Steel Housing from Palisades Nuclear Power Station:*

ID:	ANLRAP-98-92	
PI:	Luis Nuñez Chemical Technology Division	
Phone:	630 252-3069	
Partner:	Uni-Chem Chemicals, Inc. Baroda, MI	
FY99 Funding:		$5K
Total Project Funds:		$5K

Background

Decontamination activities in the nuclear industry account for a significant amount of cost and time lost during a planned or unplanned shutdown. Often contaminated equipment is stored or disposed because there is no reliable solvent that can remove the contamination effectively.

Research Objective

Argonne National Laboratory has developed a novel decontamination solvent for removing oxide scales formed on ferrous metals typical of nuclear reactor piping and housing. The decontamination process is based on the properties of the diphosphonic acids (specifically 1-hydroxyethane-1,1-diphosphonic acid or HEDPA) coupled with strong reducing agents. This solvent offers many advantages over current decontamination solvents in that it is relatively non-toxic, has low vapor pressure, does not harm the base metal, and its waste can be formed into stable metal phosphates. Recognizing the potential applications of this solvent in the nuclear industry, Uni-Chem Chemicals has collaborated with ANL to further develop the HEDPA process. The successful development and demonstration of this process will provide leverage to obtain programmatic funding through Uni-Chem Chemicals from various nuclear utilities.

Results

Consumers Energy's Palisades Nuclear Plant (Covert, MI) has a number of large radioactively contaminated components ranging from hand tools to full size steam generators. Uni-Chem Chemicals arranged for the shipment of reactor housing components from Palisades Nuclear to ANL. The components contained radioactive contamination from both neutron activation and surface scale deposits. The pieces were submerged in circulating HEDPA solution for two days. From the gamma and visual characterization of the pieces, it is evident that the HEDPA decontamination solvent was very effective, leaving background activation products as the sole source of radiation. This was verified by decontamination factor calculations, which showed the decontamination to be extremely large.

69: *Development of Techniques for Production of Nanofluids for Heat Transfer Applications*

ID:	ANL 98-SC-13	
PI:	Jeffrey Eastman Materials Science Division	
Phone:	630 252-5141	
Partner:	Nanopowder Enterprises, Inc. Piscataway, NJ	
FY 99 Funding:		$50K
Total Project Funds:		$100K

Background

Many industrial sectors, including transportation, energy supply and production, electronics, textiles, and paper production, use heating or cooling fluids in key roles. These industries have a strong need for improved fluids that can transfer heat more efficiently. Argonne is developing a new class of heat transfer fluids called "nanofluids" that transfer heat more efficiently than conventional fluids and offer several benefits, including decreased pumping power needs or reduction in required heat exchanger size. Nanofluids consist of nanometer-sized solid particles dispersed in traditional heat transfer fluids. Because solids have orders-of-magnitude greater thermal conductivities than those of fluids such as water, ethylene glycol, or oil, the solid particles substantially improve the heat transfer properties of the fluid.

Research Objective

The goals of this project are to (1) determine the thermal conductivity enhancement of several nanofluids consisting of either metallic or oxide nanoparticles dispersed in water or ethylene glycol, and (2) develop and evaluate techniques for cost-effective industrial scale production of nanofluids.

Nanofluids are produced at Argonne by the VEROS (Vacuum Evaporation onto a Running Oil Substrate) technique. Argonne is working with Nanopowder Enterprises Inc. (NEI) to determine the feasibility of adapting the VEROS technique to eventual industrial scale production rates. Nanopowder Enterprises is also investigating the feasibility of other techniques for commercial-scale production. The project extends DOE’s investments in materials characterization to further improvements in heat transfer processes which will have applications over a broad industry sector.

Results

NEI has developed a patented Combustion Flame – Chemical Vapor Condensation (CF-CVC) process to produce nanoparticles with very little aggregation. Alumina-in-water nanofluids were recently produced by NEI using this technique, and their thermal conductivities are currently being measured by Argonne. Progress has also been made recently towards the goal of incorporating a means of monitoring particle loadings during VEROS synthesis of nanofluids in real-time. A thermal conductivity apparatus has been set-up at Argonne, and initial measurements of alumina-in-water nanofluid thermal conductivities using this apparatus have been completed. This system is currently being interfaced to Argonne's VEROS system. The next goal will be to use the same apparatus to measure the thermal conductivities of fluids with systematically varying nanoparticle loadings. Then, as a final step, the results of these calibration runs will be used to determine particle loadings during processing as an in-situ process monitor.

70: *Catalyst Development and Optimization for Condensed Phase Processing*

ID:	PNL 98-SC-01	
PI:	Tod Werpy	
Phone:	509 372-4638	
Partner:	National Corn Growers Association St. Louis, MI	
FY 99 Funding:		$30K
Total Project Funds:		$30K

Background

Recent improvements in fermentation technology, molecular biology, and separations technology have made the production of chemicals from renewable feedstocks economically attractive. A new method to synthesize highly active metal dispersed catalysts, for use in condensed systems, has been developed. The catalysts have been shown to be more active toward the hydrogenation of organic acids in the condensed phase than any commercial catalyst. These catalysts afford an opportunity to develop commercially viable processes for producing chemicals from renewable feedstocks, such as corn derived glucose.

Research Objective

The goal of this project, between Pacific Northwest Laboratories and the National Corn Growers Association, is to determine optimum synthesis conditions, oxide loading, and metal loading for catalysts. Ideal properties for the catalyst would be high selectivity and conversion rates, low cost, long lifetime, and stability toward hydrolysis. The model reaction for the study is the catalytic hydrogenation of lactic acid to propylene glycol. A process economics analysis will be developed to compare new catalyst performance to commercially available ones.

Results

The new catalysts are based on a mixed system of carbon and a metal oxide that serves as the support. Active metals, such as palladium, rhodium, rhenium, and ruthenium, are impregnated on these novel supports and then screened for their activity and other desirable properties. For example, a palladium-impregnated zirconia/carbon textured catalyst has been shown to yield 50% hydrogenation in one half the time of the commercially available variety. The difference in rate indicates that diffusion limitations have been reduced in the new system. Improvements in these reductions will have a substantial effect on the capital cost of large scale conversion of renewable feedstocks. This project supports DOE initiatives for efficient energy production from alternative energy sources.

APPENDIX A

CROSS REFERENCE TABLE FOR MULTI-YEAR PROJECTS*

	National Laboratory						
Program Focus Area	**AL**	**ANL**	**BNL**	**LBL**	**ORL**	**PNL**	**SLAC**
Advanced Materials							
Design of Materials		1		2, 3, 4		5	
Advanced Synthesis and Characterization				6, 7	8	9	
Films and Coatings		10, 11, 12, 13	14	15	16, 17, 18		
Energy Conversion and Storage		19, 20,	21				
Intelligent Processing and Manufacturing Research							
Intelligent Design		22, 23			24	25, 26	
Enabling Technologies			27, 28, 29	30, 31	32		33
Environmental and Biomedical Research							
Biological and Environmental Technologies		34			35	36, 37	
Medical Technologies		38	39, 40, 41	42, 43, 44, 45	46	47	
Cleaner Industrial Processes	48	49, 50, 51	52	53	54, 55	56, 57	
Major Industry Partnerships							
Advanced Computational Technology Initiative (ACTI)		58		59, 60, 61			
American Textiles (AMTEX) Partnership		62			63, 64	65, 66	

The numbers in this table refer to the project number, which is located next to the project title. The project number is the same as the page number.

APPENDIX B

ALPHABETICAL LIST OF INDUSTRIAL PARTNERS*

*The numbers in this table refer to the project number, which is located next to the project title. The project number is the same as the page number.

APPENDIX C

ALPHABETICAL LIST OF PRINCIPAL INVESTIGATORS*

*The numbers in this table refer to the project number, which is located next to the project title. The project number is the same as the page number.